United States Patent and Trademark Office

APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
13/412,887	03/06/2012	Nigel P. Duffy	NUM011CON	5269

54698	7590	06/13/2018	EXAMINER	

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ART UNIT	PAPER NUMBER
1631	

NOTIFICATION DATE	DELIVERY MODE
06/13/2018	ELECTRONIC

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PTOL-90A (Rev. 04/07)

UNITED STATES PATENT AND TRADEMARK OFFICE

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BEFORE THE PATENT TRIAL AND APPEAL BOARD

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Ex parte NIGEL P. DUFFY[1]

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Appeal 2017-000697
Application 13/412,887
Technology Center 1600

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Before RICHARD M. LEBOVITZ, RICHARD J. SMITH, and
TIMOTHY G. MAJORS, *Administrative Patent Judges.*

SMITH, *Administrative Patent Judge.*

DECISION ON APPEAL

This is an appeal under 35 U.S.C. § 134 involving claims to a method
for training a molecular properties model and predicting a property of
interest for a test molecule. We have jurisdiction under 35 U.S.C. § 6(b).

We affirm.

STATEMENT OF THE CASE

Background

"In the fields of bioinformatics and computational chemistry, machine
learning applications have been used to develop models of various molecular

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[1] According to Appellant, the real party in interest is Numerate, Inc.
(Appeal Br. 3.)

properties. Oftentimes, such models are built in an attempt to predict whether a particular molecule will exhibit the property being modeled." (Spec. ¶ 5.)

"The training examples used to train a molecular properties model each typically include a description for a molecule . . . and data regarding the property of interest for the molecule. Collectively, the training examples are commonly referred to as a 'training set' or as 'training data.'" (*Id.* ¶ 6.)

"[I]t is often easier (and more accurate) to consider the ordering of two molecules relative to a certain property than it is to assert an absolute value for the property for a single molecule. Existing molecular property modeling techniques, however, are not capable of using such ordering information." (*Id.* ¶ 11.)

Claims on Appeal

Claims 11–23 are on appeal.[2] (Claims Appendix, Appeal Br. 12–14.) Claim 11 is the only independent claim on appeal and reads as follows:

> 11. A method for training a molecular properties model and predicting a property of interest for a test molecule, comprising, on a computer system:
> obtaining a pseudo-partial ordering of molecules represented by a set of two or more ranked pairs of molecules, wherein the molecules within the pairs are ordered relative to one another based on the property of interest that is physically testable selected from the group consisting of reactivity, binding affinity, melting point, solubility, membrane permeability, toxicity, pKa, and combinations thereof;
> generating a representation of the molecules included in the pseudo partial ordering of molecules that is appropriate for a selected machine learning algorithm;

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[2] Claims 1–10 and 24–41 are cancelled. (*See* Final Office Action dated Oct. 19, 2015 ("Final Act."), at 2.)

providing as a training set the set of pairs of the pseudo partial
ordering of molecules to the selected machine learning
algorithm that optimizes a function of the pairs, wherein
the molecules that comprise the pairs are ranked correctly
in the obtained ranked pairs relative to the property of
interest, and wherein, for at least a pair in the training set,
said function penalizes an incorrectly ordered said pair
implied by the function;

executing on the computer system the selected machine learning
algorithm to generate a trained molecular properties
model;

generating a representation of an additional molecule appropriate
for the molecular properties model, which molecule is the
test molecule; and

using the molecular properties model, generating on the
computer system a prediction of a value of the property of
interest for said test molecule; and

further comprising independent of the computer system
determining the accuracy of the prediction for said test
molecule by performing a laboratory confirmation of the
predicted property of interest using a physically realized
sample of said test molecule.

Examiner's Rejection

Claims 11–23 stand rejected under 35 U.S.C. § 101 as directed to non-statutory subject matter. (Ans. 3–4.)

DISCUSSION

Issue

Whether a preponderance of evidence of record supports the Examiner's rejection of claims 11–23 under 35 U.S.C. § 101.

Principles of Law

On issues of patent eligibility, we "first determine whether the claims at issue are directed to a patent-ineligible concept," such as laws of nature,

natural phenomena, and abstract ideas. *Alice Corp. Pty. Ltd. v. CLS Bank Int'l*, 134 S. Ct. 2347, 2355 (2014) ("*Alice*"). If this threshold is met, we move to the second step of the inquiry and "consider the elements of each claim both individually and 'as an ordered combination' to determine whether the additional elements 'transform the nature of the claim' into a patent-eligible application." *Id.* (quoting *Mayo Collaborative Servs. v. Prometheus Labs., Inc.*, 566 U.S. 66, 78–79 (2012) ("*Mayo*")).

Analysis

We adopt the Examiner's findings and conclusion that the claims are directed to non-statutory subject matter. (Advisory Action dated Jan. 20, 2016, at 2; Ans. 3–7.) We discern no error in the rejection of claims 11–23 under Section 101. We limit our consideration to claim 11 because the claims were not argued separately.

According to Appellant, claim 11 is directed to a method of determining "the properties of a molecule with a machine learning algorithm that uses ranked pairs of molecules as the training data. Using this relative ranking allows robust computer models to be constructed in situations where data sources are too noisy to allow such modeling using traditional valuations of the molecules." (Appeal Br. 3–4.)

Examiner's Position

> As to *Alice* step one, the Examiner finds that claim 11 is
>
> directed to obtaining a list of ordered molecules, generating a list of data representing the molecules, providing the "pairs of molecules" (which is in data form) to an algorithm that ranks the molecules according to a molecular property of interest, generating further data representing an additional molecule, [and] predicting information regarding the property of interest

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for the additional molecule. The method further requires a laboratory "confirmation," of the predicted information about property of interest in the additional molecule using a physical sample of the model. As a whole the method relies on the abstract ideas of comparing information, categorizing, organizing and transmitting information and organizing information through mathematical correlations.

(Ans. 3–4.)

Regarding *Alice* step two, the Examiner finds that claim 11

do[es] not include additional elements that are sufficient to amount of significantly more than the judicial exception because it is routine and conventional to perform the acts of testing a physical molecular sample to determine at least one property of the molecules. Other elements of the method include using a computer system to obtain and generate data as well as perform the algorithmic calculation. However, this is a recitation of generic computer structure that serves to perform generic computer functions that are well-understood, routine, and conventional activities previously known to the pertinent industry. Viewed as a whole, these additional claim element(s) do not provide meaningful limitation(s) to transform the abstract idea into a patent eligible application of the abstract idea such that the claim(s) amounts to significantly more than the abstract idea itself.

(*Id.* at 4.)

Based on those findings, the Examiner concludes that claim 11 is directed to non-statutory subject matter and unpatentable under Section 101. (*Id.*)

Appellant's Arguments

Appellant argues that "nothing in this record indicates that a molecular properties model based on ***ordered pairs*** of molecules is known or routine. Thus, on this record, and Applicant submits in actual fact, there is nothing routine or conventional about the claimed method." (Appeal Br. 5.)

We are not persuaded. As an initial matter, the Specification makes clear that the use of molecular properties models, training sets, and machine learning algorithms are routine and conventional in the fields of bioinformatics and computational chemistry. (*See, e.g.*, Spec. ¶¶ 5, 6.) Moreover, the Specification indicates that "any available computer system" may be used and identifies by name multiple prior learning algorithms that may be used in the claimed method. (*See* Spec. ¶¶ 29, 83.)

Regarding the use of ranked pairs of molecules ("ordered pairs") as the training data, the Examiner explains that "the molecular properties model is one based on mathematical relationships, algorithms and data. It is drawn to an abstract idea." (Ans. 6.) That is, providing training data in the form of ordered pairs involves the abstract idea of comparing, organizing, and transmitting information.[3] (*Id.* at 4.) We thus agree with the Examiner's finding because abstract ideas include collecting information and analyzing that information "by steps people go through in their minds, or by mathematical algorithms." *FairWarning IP, LLC v. Iatric Sys., Inc.*, 839 F.3d 1089, 1093 (Fed. Cir. 2016) (internal quotation marks and citation omitted). Put concisely, "[w]ithout additional limitations, a process that employs mathematical algorithms to manipulate existing information to generate additional information is not patent eligible." *Digitech Image Techs., LLC v. Elecs. for Imaging, Inc.*, 758 F.3d 1344, 1351 (Fed. Cir. 2014).[4]

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[3] A model based on ordered pairs of molecules is thus an abstract idea under *Alice* step 1. (Ans. 3–4, 6.)

[4] *See also Intellectual Ventures I LLC v. Capital One Fin. Corp.*, 850 F.3d 1332, 1340 (Fed. Cir. 2017), discussing cases in which claims reciting data manipulation steps were held to be patent ineligible as abstract ideas.

Appellant argues that the claimed invention improves the functioning of the computer. (Appeal Br. 6–8.) In advancing that argument, Appellant characterizes the invention as a form of digital image processing of the type that was found patent eligible in *Research Corp. Techs., Inc. v. Microsoft Corp.*, 627 F.3d 859 (Fed. Cir. 2010).[5] (*Id.* at 6.) Appellant also relies on the Supplemental Allgood Declaration[6] to support the contention that the claimed invention improves the functioning of the computer. (*Id.* at 7.) According to Appellant, "the claimed method using ordered pairs improves the method of visualizing the activity of molecules." (*Id.*)

We are not persuaded. As explained by our reviewing court in *Bancorp Servs., L.L.C. v. Sun Life Assur. Co. of Canada (U.S.)*, 687 F.3d 1266, 1279 (Fed. Cir. 2012), "the claimed processes in *Research Corp.* plainly represented improvements to computer technologies in the marketplace," such as the use of an inventive mask that produced "higher quality halftone images while using less processor power and memory space." (*Id.*, quoting *Research Corp.*, 627 F.3d at 865.) As further explained in *Bancorp*, the method in *Research Corp.* "required the manipulation of computer data structures . . . and the output of a modified computer data structure . . . dependent upon the computer components required to perform it." *Id.*

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[5] Appellant references Example 3 of EXAMPLES: ABSTRACT IDEAS issued by the USPTO on January 27, 2015, rather than *Research Corp.*, but that Example 3 was based on the *Research Corp.* decision. *See id.* at 7–10 (https://www.uspto.gov/sites/default/files/documents/abstract_idea_examples.pdf).
[6] Supplemental Declaration Under 37 C.F.R. § 1.132 of Brandon Allgood, dated Dec. 18, 2015 ("Allgood Declaration" or "Decl.").

Here, the focus of claim 11 is not to any improved computer, but rather to an improved mathematical analysis, and the Specification states that readily available computer technology is usable to carry out the analysis. *See SAP Am., Inc. v. Investpic, LLC*, 890 F.3d 1016, 1023 (Fed. Cir. 2018). Stated another way, claim 11 is not directed to a physical-realm improvement, "but an improvement in wholly abstract ideas—the selection and mathematical analysis of information, followed by reporting or display of the results." *Id.* at 1022. Moreover, given Appellant's contention that "[t]he invention is to a method of determining the properties of a molecule with a machine learning algorithm that uses ranked pairs of molecules as the training data" (Appeal Br. 4), we find that the recited generic computer elements "'are invoked merely as a tool.'" *Credit Acceptance Corp. v. Westlake Servs.*, 859 F.3d 1044, 1055 (Fed. Cir. 2017) (quoting *Enfish, LLC v. Microsoft Corp.*, 822 F.3d 1327, 1335–36 (Fed. Cir. 2016)).

The Allgood Declaration does not change this analysis. Rather than describing an actual improvement to a computer itself, the Allgood Declaration states that the use of ordered pairs of molecules "provides for more robust input, resulting in better models and better predictions." (Decl. ¶ 4.) That statement does not describe an improvement to the computer itself, but (at most) an improvement in wholly abstract ideas. *See SAP*, 890 F.3d at 1022.

Appellant argues that "these predictions with ordered pairs is [not] in the prior art," "an important invention is achieved" by the claims, and that "[o]ne is not monopolizing the field of computational chemistry, as conventional methods work." (Appeal Br. 7–8.) We are not persuaded. It is not enough for subject-matter eligibility that a claimed method be novel and

nonobvious in light of prior art. *See SAP*, 890 F.3d at 1018; *Synopsys, Inc. v. Mentor Graphics Corp.*, 839 F.3d 1138, 1151 (Fed. Cir. 2016) ("a claim for a *new* abstract idea is still an abstract idea"). Moreover, even if the claimed method is "brilliant," "innovative," or "groundbreaking," that is not enough for eligibility. *See SAP*, 890 F.3d at 1018 (internal citations, quotations, and alteration omitted). Furthermore, the alleged lack of "monopolizing the field" is unpersuasive because "the absence of complete preemption does not demonstrate patent eligibility." *Ariosa Diagnostics, Inc. v. Sequenom, Inc.*, 788 F.3d 1371, 1379 (Fed. Cir. 2015).

Appellant also relies on *DDR Holdings, LLC v. Hotels.com, L.P.*, 773 F.3d 1245, 1257 (Fed. Cir. 2014), and the argument that the solution of claim 11 is "necessarily rooted in computer technology." (*See* Appeal Br. 10, quoting *DDR Holdings*.) However, as explained by our reviewing court, the focus of the claims in *DDR Holdings* was to an improvement to computer functionality itself, rather than simply the use of computers. *Affinity Labs of Tex., LLC v. DIRECTV, LLC*, 838 F.3d 1253, 1261–62 (Fed. Cir. 2016) (distinguishing *DDR Holdings*). Moreover, rather than being rooted in computer technology, the claims at issue here simply use computer technology "as tools in the aid of a process focused on an abstract idea." *Id.* at 1262.

Appellant's Reply Brief cites to *Enfish* and *McRO, Inc. v. Bandai Namco Games Am. Inc.*, 837 F.3d 1299 (Fed. Cir. 2016) as support for the proposition that "when the invention improves the operation of a computer or relevant technology with a specific means or method, you do not even have an abstract idea exception for which you need to seek 'something more.'" (Reply Br. 3.) Even if we accept Appellant's characterization of

McRO and *Enfish*, claim 11 is not directed to the improved operation of a computer but to a claimed improvement to "the selection and mathematical analysis of information, followed by reporting or display of the results." *See SAP*, 890 F.3d at 1022 (distinguishing *McRO* and *Enfish*); *see also Elec. Power Grp., LLC v. Alstom S.A.*, 830 F.3d 1350, 1353–54 (Fed. Cir. 2016) ("collecting information, analyzing it, and displaying certain results of the collection and analysis" "fall[s] into a familiar class of claims 'directed to' a patent-ineligible concept," that of the abstract idea) (distinguishing claims in *Enfish*).

Accordingly, for the reasons of record and as set forth above, we affirm the rejection of claim 11 as being directed to a judicial exception without significantly more, and thereby being directed to non-statutory subject matter under 35 U.S.C. § 101. Claims 12–23 fall with claim 11 because they were not argued separately.

Conclusion

A preponderance of evidence of record supports the Examiner's rejection of claims 11–23 under 35 U.S.C. § 101.

SUMMARY

We affirm the rejection of all claims on appeal.

TIME PERIOD FOR RESPONSE

No time period for taking any subsequent action in connection with this appeal may be extended under 37 C.F.R. § 1.136(a).

AFFIRMED