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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
13/079,489	04/04/2011	Richard A. Friesner	17367-0015001	9846

26161 7590 09/10/2018
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EXAMINER

BORIN, MICHAEL L

ART UNIT	PAPER NUMBER
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1631

NOTIFICATION DATE	DELIVERY MODE
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09/10/2018

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UNITED STATES PATENT AND TRADEMARK OFFICE

BEFORE THE PATENT TRIAL AND APPEAL BOARD

Ex parte RICHARD A. FRIESNER and ROBERT MURPHY¹

Appeal 2018-005300
Application 13/079,489
Technology Center 1600

Before JEFFREY N. FREDMAN, RYAN H. FLAX, and
TIMOTHY G. MAJORS, *Administrative Patent Judges*.

FLAX, *Administrative Patent Judge*.

DECISION ON APPEAL

This is a decision on appeal under 35 U.S.C. § 134(a) involving claims directed to a method of scoring binding affinity of a plurality of proposed ligand molecules for a receptor molecule using a computer and computer databases. Claims 1 and 2 are on appeal as rejected under 35 U.S.C. § 101. We have jurisdiction under 35 U.S.C. § 6(b).

We reverse.

¹ Appellants identify the Real Party in Interest as “Schrödinger, Inc.”
Appeal Br. 1.

STATEMENT OF THE CASE

Claims 1, the sole independent claim, is representative:

1. A method of scoring binding affinity of a plurality of proposed ligand molecules for a receptor molecule using a computer and computer data bases, the receptor being a protein, method comprising:
 - a) obtaining computer stored data representing a predicted ligand-receptor structure,
 - b) assigning a penalty to be added to the binding affinity score by computerized operations which includes the following steps:
 - i. determine whether a dissociated receptor of the predicted ligand-receptor structure includes localized solvating water molecule(s) that a) are proximate to a formally charged group of the receptor and b) have a larger occupancy density at the hydration site compared to the number density of bulk solvent, and c) form hydrogen bonds with a charged atom of an amino acid residue in a side chain of the receptor protein, whereby desolvation of said localized solvating water molecules into the surrounding environment requires energy,
 - ii. determine whether the configuration of the receptor-ligand complex requires desolvation of one or more of the localized solvating water molecule(s) referred to above in (i), and, if so,
 - iii. assign a desolvation penalty to be added to the binding affinity score of the ligand provided, however, that the scoring includes determining whether a charged atom of the amino acid residue that includes the side chain atom is in a salt bridge with an oppositely charged receptor atom,

and, if so, the penalty is not assessed,

identifying one or more active complexes based on the scored binding affinities for the plurality of proposed ligand molecules and receptor molecule; and

testing a proposed ligand molecule of at least one of the identified active complexes, wherein the scored binding affinities discriminate one or more inactive complexes to facilitate screening the plurality of proposed ligand molecules for binding to the receptor molecule.

Appeal Br. 11–12 (Claims Appendix).

The following rejections are appealed:

Claims 1 and 2 stand rejected under 35 U.S.C. § 101 as directed to patent-ineligible subject matter. Final Action 3.

DISCUSSION

“[T]he examiner bears the initial burden, on review of the prior art *or on any other ground*, of presenting a *prima facie* case of unpatentability. If that burden is met, the burden of coming forward with evidence or argument shifts to the applicant.” *In re Oetiker*, 977 F.2d 1443, 1445 (Fed. Cir. 1992) (emphasis added).

“Phenomena of nature, though just discovered, mental processes, and abstract intellectual concepts are not patentable, as they are the basic tools of scientific and technological work.” *Mayo Collaborative Servs. v. Prometheus Labs, Inc.*, 566 U.S. 66, 71 (2012) (quoting *Gottschalk v. Benson*, 409 U.S. 63, 67 (1972)). Claims directed to *nothing more than* abstract ideas (such as mathematical algorithms), natural phenomena, and laws of nature are not eligible for patent protection. *Diamond v. Diehr*, 450 U.S. 175, 185 (1981); accord MPEP § 2106 (II) (discussing *Diehr*); *see also*

Parker v. Flook, 437 U.S. 584, 592–94 (1978) (if, once the mathematical algorithm is removed from consideration, nothing patentable remains, the claims are not patent-eligible).

In analyzing patent-eligibility questions under 35 U.S.C. § 101, the Supreme Court instructs us to “first determine whether the claims at issue are directed to a patent-ineligible concept.” *Alice Corp. Pty. Ltd. v. CLS Bank Int’l*, 134 S. Ct. 2347, 2355 (2014). If the claims are so-directed, we then move to a second step 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*, 566 U.S. at 78–79).

Here, under *Alice*’s step one, the Examiner determined,

The claims are directed to a process, which is one of statutory categories of invention. The process is a computational method of calculating a corrected binding score of ligand-receptor complex. The claimed invention comprises the steps of calculating a desolvation penalty to be applied to a score representing binding affinity of ligand to receptor. As such, the claims are drawn to processing information, converting one form of numerical representation into another by organizing information through mathematical concepts, and applying rules and categorizing information. Thus, the claims are directed to an abstract idea which is a judicial exception.

Final Action 3. Under *Alice*’s step two, the Examiner determined that “[t]he claims do not include additional elements that are sufficient to amount to significantly more than the judicial exception,” noting specifically,

The claims further address a step of testing of a ligand. The testing does not address any particular ligand, but rather – any ligand from active ligand-receptor complexes. Further, the “testing” is not viewed as *in vitro*: based on specification, the

“testing” is *in silico* testing of scoring functions. Paragraph [058]). Even if specification had support for *in vitro* testing, such testing [for an unidentified characteristics] consist of well-understood, routine, conventional activity of ligand testing already engaged in by the scientific community. Essentially, appending conventional steps, specified at a high level of generality, to a judicial exemption, such as abstract ideas, cannot make these ideas patent-eligible.

Id. at 3–4 (brackets in original).

It is without question that “[t]he line between a patentable ‘process’ and an unpatentable ‘principle’ is not always clear.” *Flook*, 437 U.S. at 589; *see also Synopsys, Inc. v. Mentor Graphics Corp.*, 839 F.3d 1138, 1150 (Fed. Cir. 2016) (“defining the precise abstract idea of patent claims in many cases is far from a ‘straightforward’ exercise”) (quoting *DDR Holdings, LLC v. Hotels.com, L.P.*, 773 F.3d 1245, 1257 (Fed. Cir. 2014)). Here, a reasonable case could be made that the Examiner’s determination under *Alice*’s step one is without error on the basis that the claims are directed to the manipulation of data using mathematical algorithms. *See Intellectual Ventures I LLC v. Capital One Financial Corporation*, 850 F.3d 1332, 1339–40 (2017) (claims were held to be directed to a computer programmed to edit XML documents, which the Federal Circuit “conclude[d] [were] . . . at their core, directed to the abstract idea of collecting, displaying, and manipulating data”); *see also Electric Power Grp., LLC v. Alstom S.A.*, 830 F.3d 1350 (Fed. Cir. 2016). On the other hand, a reasonable case could also be made that that the claims are not directed to a mere abstract idea, even though they are software-based and relate to mathematical calculations, because the claimed method solves a problem in an existing technical field using a set of rules-based steps. *See McRO, Inc. v. Bandai Namco Games*

America Inc., 837 F.3d 1299 (Fed. Cir. 2016); *see also Trading Technologies International, Inc. v. CQG, INC.*, 675 Fed. Appx. 1001 (Fed. Cir. 2017).

Even if the claims on appeal are “directed to” an abstract idea under the first step of the *Alice* framework as determined by the Examiner, we conclude that the Examiner has not established that the additional elements recited in the claims, considered individually and as an ordered combination, were well-understood, routine, and conventional as required under the second step of *Alice*. Regarding the Examiner’s determination that the non-abstract-idea claim elements are merely routine and conventional, the Federal Circuit has explained that

Whether something is well-understood, routine, and conventional to a skilled artisan at the time of the patent is a factual determination. Whether a particular technology is well-understood, routine, and conventional goes beyond what was simply known in the prior art. The mere fact that something is disclosed in a piece of prior art, for example, does not mean it was well-understood, routine, and conventional.

Berkheimer v. HP Inc., 881 F.3d 1360, 1369 (Fed. Cir. 2018).

Here, the Examiner identified that the claims require a ligand testing step and concluded that “such testing [for unidentified characteristics] consist of well-understood, routine, conventional activity.” Final Action 4. However, the Examiner has identified no evidence to support this conclusion. For this reason, we find the rejection insufficient.

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SUMMARY

The rejection of the claims as directed to patent-ineligible subject matter is reversed.

REVERSED