CARBONS INTO BYTES: PATENTED CHEMICAL COMPOUND PROTECTION IN THE VIRTUAL WORLD

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ABSTRACT

"Virtual" molecular compounds, created in molecular modeling software, are increasingly useful in the process of rational drug design. When a physical compound is patented, however, virtual use of the compound allows researchers to circumvent the protection granted to the patentee. To acquire protection from unauthorized use of compounds in their virtual form, patentees must directly claim the virtual compound. But Supreme Court decisions such as Bilski v. Kappos *and* Mayo Collaborative Services v. Prometheus Laboratories, Inc. *call into question whether virtual compound claims are patentable subject matter under § 101. Using the guidance offered by the Supreme Court and Federal Circuit, this Issue Brief argues that virtual compound claims are not abstract ideas and therefore, consistent with patent policy, qualify as patentable subject matter.*

INTRODUCTION

In 2000, the estimated cost of developing a new drug was $802 million.[1] More recent estimates suggest the sum is actually around $2 billion.[2] A large proportion of this cost involves identifying a substance that shows promise as a starting point for a new drug. This substance is identified in drug discovery as the lead compound.[3]

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[1] Joseph A. DiMasi, Ronald W. Hansen & Henry G. Grabowski, *The Price of Innovation: New Estimates of Drug Development Costs*, 22 J. HEALTH ECON. 151, 166 (2003).

[2] Neal Masia, *The Cost of Developing a New Drug*, *in* FOCUS ON: INTELLECTUAL PROPERTY RIGHTS 82, 82 (U.S. Dep't of State ed., 2006), *available at* http://photos.state.gov/libraries/amgov/30145/publications-english/iprbook.pdf.

[3] AHINDRA NAG & BAISHAKHI DEY, COMPUTER-AIDED DRUG DESIGN AND DELIVERY SYSTEMS 4 (2011).

Following the discovery of the lead compound, the traditional method of drug design involves consistently altering the lead compound to identify a safe and potent compound worth the expense of clinical trials.[4] However, even after identifying a lead compound, the odds are still 1 in 10,000 that drugs identified as "promising" will result in a commercialized product.[5] In fact, the primary expenditure in drug design is failure.[6]

The traditional method of drug design requires iterating through possibly thousands of compounds in the search for a commercially viable drug.[7] This process is expensive in both labor and equipment.[8] One study showed that this "discovery phase" incurs 68 percent of the actual cost for each drug placed on the market for consumers.[9] Costs increase even more if a company has to license the lead compound from a patentee to perform experiments.[10]

The use of computer-aided drug design employing computational chemistry reduces experimentation costs by eliminating the need for multiple, repetitive reactions.[11] In the 1990s and early 2000s, the pharmaceutical industry believed that the possibility of generating virtual lead compounds entirely through computer simulation, known as *de novo* design, would revolutionize the industry.[12] Unfortunately, limitations in

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[4] *Id.*

[5] RICHARD B. SILVERMAN, THE ORGANIC CHEMISTRY OF DRUG DESIGN AND DRUG ACTION 8 (2d ed. 2004).

[6] Matthew Herper, *The Truly Staggering Cost of Inventing New Drugs*, FORBES, (Feb. 10, 2012, 7:41 AM), http://www.forbes.com/sites/matthewherper/2012/02/10/the-truly-staggering-cost-of-inventing-new-drugs/.

[7] NAG & DEY, *supra* note 3, at 2.

[8] *Id.*

[9] *See id.* While this study valued the total cost for each drug placed on the market for consumers lower than other estimates, it estimated that $156 million of the $231 million cost for each drug placed on the market for consumers is in discovering the compound.

[10] *See* 35 U.S.C. § 271(a) (2012) ("[W]hoever without authority makes, uses, offers to sell, or sells any patented invention . . . infringes the patent."). *But see* 35 U.S.C. § 271(e) (2012) (permitting, under the experimental-use exception, unauthorized uses for purposes "reasonably related to the development and submission of information under a Federal law which regulates the manufacture, use, or sale of drugs or veterinary biological products")

[11] NAG & DEY, *supra* note 3, at 9; *see also* Bruce R. Gelin, *Current Approaches in Computer-Aided Molecular Design*, *in* COMPUTER-AIDED MOLECULAR DESIGN: APPLICATIONS IN AGROCHEMICALS, MATERIALS AND PHARMACEUTICALS 1, 5 (Charles H. Reynolds et al. eds., 1995).

[12] NAG & DEY, *supra* note 3, at 9.

computing power limited the effectiveness of *de novo* design.[13] Many in the industry deemed *de novo* design a failure.[14]

Despite some of the historical failures and concerns surrounding computer-aided drug design, patent practitioners need be aware of the patent issues surrounding virtual compounds because of their current and possible future role in drug design. Rapid advances in computing power make it reasonably likely that in the future, *de novo* design will become a viable mode of drug design. And in the mean time, another technique utilizing virtual compounds, known as *drug optimization*, still makes virtual-compound patent concerns relevant.[15]

Whereas *de novo* design begins the entire process from mere theoretical knowledge, *drug optimization*, like the traditional method, begins with a previously identified lead compound. The structure of that compound, bound with its receptor, is analyzed by x-ray crystallography.[16] The potency of the lead compound is then optimized by generating and predicting the binding of potential derivatives using mass screening and combinatorial chemistry.[17]

Unlike the traditional method, however, drug optimization does not use the actual compound. Therefore, a company may not need to license the lead compound from the patentee for purposes of virtual experimentation. On the other hand, any claim directed to the compound in virtual form would likely come under § 101 scrutiny as to whether or not the claim is patentable subject matter, especially given the recent Supreme Court cases *Bilski v. Kappos*[18] and *Mayo Collaborative Services v. Prometheus Laboratories, Inc.*[19]

This Issue Brief proceeds in two Parts. Part I addresses whether or not patents on lead compounds protect the patentee from unauthorized use of the compounds in virtual form. Part II analyzes the current law to determine whether virtual compound claims are patentable subject matter. A brief Conclusion follows.

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[13] *Id.*
[14] *Id.*
[15] *Id.* at 9–10.
[16] *Id.*
[17] *Id*.
[18] *See* Bilski v. Kappos, 130 S. Ct. 3218 (2010) (holding that a patent application claiming a method for hedging losses by making investments in other segments of industry was invalid on the basis that the investment strategy was not patentable subject matter).
[19] *See* Mayo Collaborative Servs. v. Prometheus Laboratories, Inc, 132 S. Ct. 1289 (2012) (holding that a patent application claiming a method for using the measurement of metabolites of an applied drug to decide whether to increase or decrease drug dosage was not patentable subject matter).

I. INFRINGEMENT

Suppose Researcher *A* develops lead compound *X* in the laboratory and patents it. During the lifetime of that patent, Researcher *B* uses *X* under the traditional method to find the most promising alteration, drug *Y*. Assuming Researcher *B* has no license to use *X*, he has infringed Researcher *A*'s patent.[20]

Now imagine that instead of using the traditional method of drug design, Researcher *B* used Researcher *A*'s patent to input the spatial coordinates of compound *X* into molecular modeling software. Using computer-aided drug design, Researcher *B* is quickly able to determine the reactivity of *X* with other compounds and simulates reactions of *X* until she finds the most promising alteration, drug *Y*. In this case, there is no infringement.

Why the difference? The United States Patent Act provides that patent infringement occurs when anyone "without authority makes, uses, offers to sell, or sells any patented invention, within the United States . . . during the term of the patent therefor."[21] A court determines whether infringement has occurred using a "two-step analysis": First, it construes the claim in question to determine its scope and meaning; and second, it compares the construed claim to the invention accused of infringement.[22] For a typical compound claim, a court would likely find that there is no infringement.[23]

A. Prong One: Claim Construction

The claim-construction prong of the test is specific to the actual claim being litigated. When construing claims, the court initially examines intrinsic evidence, such as the patent's specification and prosecution history.[24] In the absence of a novel meaning to a claim term, the court gives claim terms their ordinary meaning to one skilled in the art.[25]

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[20] *See* Madey v. Duke Univ., 307 F.3d 1351, 1362 (Fed. Cir. 2002) (holding that uses with "the slightest commercial implication" are disqualified from the common law experimental-use exception).
[21] 35 U.S.C. § 271(a) (2012).
[22] Tate Access Floors, Inc. v. Maxcess Techs., Inc., 222 F.3d 958, 964 (Fed Cir. 2000).
[23] The patent infringement analysis would be similar even if the patent claimed the atomic coordinates of the compound instead of just the compound itself. *See* Ted L. Field, Comment, *Computer-Aided Drug Design Using Patented Compounds: Infringement in Cyberspace*?, 34 J. MARSHALL L. REV. 1001, 1018 (2001).
[24] Victronics Corp. v. Conceptronic, Inc., 90 F.3d 1576, 1582–84 (Fed. Cir. 1996).
[25] Phillips v. AWH Corp., 415 F.3d 1303, 1321 (Fed. Cir. 2005).

For purposes of this analysis, assume that the claim for the patented compound *X* reads, "A *compound* of [a given] formula . . . or a pharmaceutically acceptable salt, wherein [lists elements]."[26] The words in play would be "compound" and "pharmaceutically acceptable salt," though terms such as "composition" or "crystal" are often used as well. Here, assume there are no specific definitions in the intrinsic evidence for the terms "compound" or "pharmaceutically acceptable salt." Accordingly, the court would refer to the ordinary meaning of the term "compound," for example, "substances occurring naturally or produced artificially by the reaction of two or more ingredients."[27] Similarly, a court could define a "pharmaceutically acceptable salt" as "any salt derived from a pharmaceutically acceptable inorganic or organic acid or base."[28]

B. Prong Two: Comparison of the Claim to the Infringing Invention

For an accused invention to infringe a patent claim, the fact-finder must find that it embodies "every limitation of the patent claim."[29] Assume that Researcher *B* created a virtual representation of the compound patented above. Researcher *B* did not make a "compound" or a "pharmaceutically acceptable salt" but instead made a representation of the compound using information disclosed by the patent. A patent on a compound protects only the actual compound and not a representation of that compound.[30] Therefore, the virtual compound does not embody every (or even any) element of the claim, making it likely that the factfinder would find that Researcher *B* did not directly infringe on the patented compound *X*.

C. Infringement Under the Doctrine of Equivalents

Researcher *A* might still argue that Researcher *B*'s use of the patented compound *X* in virtual form is infringing, under the doctrine of equivalents. This doctrine is based on the idea that "if two devices do the same work in substantially the same way, and accomplish substantially the

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[26] *See, e.g.*, U.S. Patent No. 8,263,585, claim 1 (issued Sept. 11, 2012).
[27] *E.g.*, Pharmacia Labs. Inc. v. U. S., 609 F.2d 491, 493 n.3 (C.C.P.A. 1979) (providing the definition from the Tariff Schedules of the U.S. Annotated).
[28] *E.g.,* U.S. Patent No 7,138,404 col. 3:56–58 (filed Nov. 21, 2006) (providing a definition for the term as used in this patent).
[29] Tate Access Floors, Inc. v. Maxcess Techs., Inc., 222 F.3d 958, 964 (Fed. Cir. 2000).
[30] *In re* Papesch, 315 F.2d 381, 391 (C.C.P.A. 1963). Judge Rich wrote that "the graphic formulae [and] the chemical nomenclature . . . are symbols by which compounds can be identified, classified, and compared. But a formula is not a compound and while it may serve in a claim to identify what is being patented, as the meted and bounds of a deed identify a plot of land, the thing that is patented is not the formula but the compound identified by it." *Id.*

same result, they are the same, even though they differ in name, form or shape."[31]

One of the generally accepted tests for equivalence—implementing this general principle—is the function-way-result test.[32] Under this test, each element of the claim must be examined to determine whether the accused compound performs substantially the same function, in substantially the same way, and accomplishes substantially the same result as the claimed compound.[33] The test of equivalence is applied to the "individual elements of the claim, not to the invention as a whole."[34]

There is at least a colorable argument that the computer representation embodies an equivalent of each element in the patent claim. The Federal Circuit has found that software implementations of similar functionality are equivalent: "[i]ndeed, we have upheld determinations of equivalence on the ground that hardware and software implementations of a component of an invention are interchangeable substitutes."[35] According to this argument, each virtual atom does the same thing as the physical atoms of the physical compound by interacting with virtual atoms of candidate drug molecules. Each virtual atom interacts the same way according to known laws of chemistry and physics, and each virtual atom achieves the same result by helping determine how candidate drug molecules will react with the patented compound.[36]

Another test for equivalence is the "insubstantial differences" test, which asks if there was "only an insubstantial change" in the element.[37] Under this test, Researcher *A* could argue that the difference between the actual patented compound and the virtual compound is insubstantial, given that the atoms are positioned in the same position relative to each other in both, and that the virtual compound's use is practically identical to the patented compound's use. Likewise, *A* might argue that the difference relates to the form, rather than the function, of the compound, because whether or not the compound is virtual or physical, it contains the same

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[31] Graver Tank & Mfg. Co. v. Linde Air Prods. Co., 339 U.S. 605, 608 (1950).
[32] *See id.* This test is also known as the "triple identity test." *See, e.g.*, Roger Barrett, *Discretionary Use of the Doctrine of Equivalents in Patent Law: Going Beyond the Triple Identity Test of* Graver Tank, 17 U. HAW. L. REV. 513 (1995).
[33] *Graver Tank*, 339 U.S. at 608.
[34] Warner-Jenkinson Co. v. Hilton Davis Chem. Co., 520 U.S. 17, 29 (1997).
[35] Interactive Pictures Corp. v. Infinite Pictures, Inc., 274 F.3d 1371, 1383 (Fed. Cir. 2001).
[36] Field, *supra* note 23.
[37] Hilton Davis Chem. Co. v. Warner-Jenkinson Co., Inc., 62 F.3d 1512, 1517 (Fed. Cir. 1995), *rev'd on other grounds*, Warner-Jenkinson Co. v. Hilton Davis Chem. Co., 520 U.S. 17, 29 (1997).

spatial coordinates of atoms and they react in the exact same way.[38] It would, after all, be unjust for the competitor to "exploit the . . . significant efforts and costs incurred by the patentee . . . in identifying, isolating, and effectively producing [the compound]."[39]

Despite these arguments, a court would likely not find equivalence between the use of computer representations of atoms and the patented compound itself.[40] A court would almost certainly reject equivalence under the function-way-result test given that the arrangement and interaction of elements in the virtual compound do not follow the laws of chemistry and physics like the arrangement of elements in the real patented compound.[41] Instead, they interact according to a pre-programmed mathematical algorithm that *simulates* those laws using today's imperfect models.[42] Similarly, a court using the insubstantial-differences test would reject equivalence because of the fundamental difference between the composition of actual and virtual compounds. The claims at issue here require actual compounds composed of actual atoms. The virtual representations of the patented compound are fundamentally different from the physical compound itself—the latter actually reacts and is composed of the specific atoms, whereas the former is merely a software representation that reacts with other software representations.

II. THE VIRTUAL FORM OF A CHEMICAL COMPOUND UNDER § 101

Given that a patent does not protect a compound from the use of its spatial coordinates in a computer system, it might seem obvious that the way to protect the compound from virtual use is to patent the virtual compound itself. However, *Bilski* and other recent Federal Circuit and Supreme Court cases may call into question the patentability of such claims under § 101.

Section 101 defines patentable subject matter to include "process[es], machine[s], manufacture[s], and composition[s] of matter."[43] The text of § 101 also states that a claim falling into "any" one of these categories satisfies the subject-matter requirement.[44] The USPTO's guidelines elaborate on these criteria: A claimed invention "(1) must be

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[38] *See* Trevor J. Smedley & Ross A. Dannenberg, *Enforceability of Machine Patents in Virtual Worlds*, 13 J. INTERNET L. 1, 16–17 (2010) (arguing that in a virtual world a virtual mousetrap is equivalent to a real one).

[39] Jeffrey P. Kushan, Comment, *Protein Patents and the Doctrine of Equivalents: Limits on the Expansion of Patent Rights*, 6 HIGH TECH. L.J. 109, 111 (1991).

[40] *See* Field, *supra* note 23, at 1018.

[41] *See* NAG & DEY, *supra* note 3, at 9.

[42] *Id.*

[43] 35 U.S.C. § 101 (2012).

[44] *Id.*

directed to one of the four statutory categories, and (2) must not be wholly directed to subject matter encompassing a judicially recognized exception."[45] These judicial exceptions include abstract ideas, physical phenomena, and laws of nature.[46] Therefore, to determine the patentability of virtual compounds, a court must determine first, which of the statutory categories they fall within, and second, whether claims directed to virtual compounds are abstract ideas.

Virtual compound claims can be phrased to fit in many of the statutory categories; frequently, they are phrased as process claims.[47] It can be more difficult to determine whether such a claim is directed to an abstract idea,[48] but the Supreme Court's application of the "inventive concept" test in *Prometheus* provides some guidance.[49] When a claim applies a law of nature or an abstract idea "to a known structure or process,"[50] the Court has insisted that it "contain other elements or a combination of elements . . . sufficient to ensure that the patent in practice amounts to significantly more than a patent upon the natural law itself."[51] When a claim contains such additional elements, they constitute an "inventive step" that makes it patent-eligible.[52]

A. Computer-Implemented Claims and Abstract Ideas

Virtual compounds are by nature intangible and exist only in a digital environment. Seemingly the epitome of an "abstract" idea, the only thing concrete or real about a virtual compound is the computer running the simulation and the projected image on the screen. While computer programs

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[45] U.S. PAT. & TRADEMARK OFFICE, U.S. DEP'T OF COMMERCE, MANUAL OF PATENT EXAMINING PROCEDURE § 2106 (8th ed., 9th rev. Aug. 2012) [hereinafter MPEP].

[46] Diamond v. Diehr, 450 U.S. 175, 185 (1981).

[47] For an example of a process claim, see *infra* notes 83–84 and accompanying text.

[48] Even the Federal Circuit has difficulty applying the Supreme Court's standards in this determination. For examples of the Supreme Court recently vacating or reversing Federal Circuit decisions, see Mayo Collaborative Servs. v. Prometheus Labs., Inc., 132 S. Ct. 1289 (2012); WildTangent, Inc. v. Ultramercial, LLC, 132 S. Ct. 2431 (2012), *granting cert.*, *vacating and remanding* Ultramercial, LLC v. Hulu, LLC, 657 F.3d 1323 (Fed. Cir. 2011); Bilski v. Kappos, 130 S. Ct. 3218, 3225 (2010).

[49] *Prometheus*, 132. S. Ct. at 1294.

[50] *Id.* (quoting *Diehr*, 450 U.S. at 187).

[51] *Id.* (citing Parker v. Flook, 437 U.S. 584, 594 (1978); *Bilski*, 130 S. Ct. at 3230).

[52] *Id*.

per se are abstract and non-patentable,[53] many computer-implemented processes have been found to be patentable subject matter.[54]

To determine whether a claim is directed to an abstract idea, the Federal Circuit created the machine-or-transformation test, under which "[a] claimed process is surely patent-eligible under § 101 if: (1) it is tied to a particular machine or apparatus, or (2) it transforms a particular article into a different state or thing."[55] The Supreme Court has held that the "machine-or-transformation test" is an "important clue"—though not dispositive—to the patentability of a process.[56] Using this test, the question for many inventions has become: "[I]s a general-purpose computer a 'specific machine'"?[57]

A general-purpose computer can qualify as a specific machine under the machine-or-transformation test. However, the connection to the physical world provided by the computer is not enough, by itself, to transform an abstract concept into patentable subject matter.[58] Instead, the addition of a machine must "impose a meaningful limit on the scope of a claim," and "play a significant part in permitting the claimed method to be performed."[59] In the 1994 case *In re Alappat*, the Federal Circuit held that a general-purpose computer turns into a specially programmed computer once programmed with specific software.[60] Therefore, specially programmed computers impose a meaningful limit on the claim and likely satisfy the machine prong of the test.[61]

Alternatively, to pass the transformation prong of the machine-or-transformation test, the process must transform an article into a different state.[62] Often, the courts look to see whether the process can be performed mentally.[63] In *Gottschalk v. Benson*, for example, the Supreme Court found that a method of programming a general-purpose computer to convert binary-coded numbers into pure binary through a mathematical algorithm

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[53] *See* MPEP § 2106; *see also* Gottschalk v. Benson, 409 U.S. 63, 72 (1972).
[54] *See*, *e.g.*, Research Corp. Techs., Inc. v. Microsoft Corp., 627 F.3d 859, 868 (Fed. Cir. 2010); *In re* Alappat, 33 F.3d 1526 (Fed. Cir. 1994).
[55] *In re* Bilski, 545 F.3d 943, 954 (Fed. Cir. 2008).
[56] Bilski v. Kappos 130 S. Ct. 3218, 3227, 3235 (2010) (Stevens, J., concurring); *id.* at 3258 (Breyer, J., concurring).
[57] Mark A. Lemley et al., *Life After* Bilski, 63 STAN. L. REV. 1315, 1323 (2011).
[58] Fort Props., Inc. v. Am. Master Lease LLC, 671 F.3d 1317, 1322 (Fed. Cir. 2012).
[59] SiRF Tech., Inc. v. Int'l Trade Comm'n, 601 F.3d 1319, 1333 (Fed. Cir. 2010).
[60] *In re* Alappat, 33 F.3d 1526, 1545 (Fed. Cir. 1994).
[61] *See id.*
[62] *In re* Bilski*,* 545 F.3d 943, 954 (Fed. Cir. 2008).
[63] *See*, *e.g.*, Gottschalk v. Benson*,* 409 U.S. 63, 67, 71–72 (1972); CyberSource Corp. v. Retail Decisions, Inc., 654 F.3d 1366, 1375 (Fed. Cir. 2011).

was not patent-eligible because the calculations could be performed mentally.[64]

By contrast, in *SiRF Technology, Inc. v. International Trade Commission*, the Federal Circuit found that a process was patentable because the calculations to determine the position of a GPS receiver could not be performed entirely by the human mind.[65] Similarly, the Federal Circuit in *Research Corp. Technologies, Inc. v. Microsoft Corp.* found that a method that manipulated computer data structures (like pixels of a digital image) and output a modified computer data structure was patentable subject matter.[66] Since the human mind could not practically perform this entire function, the Federal Circuit found that the transformation of the computer data structures into a different data structure was not an abstract idea.[67]

In the same vein and for the same purpose as the mental-process inquiry, courts look to see how integral a machine is to the performance of the claim. The process claimed in *SiRF* was patentable subject matter because it was impossible to generate ranges necessary to determine the position of the GPS receiver without the use of a GPS receiver.[68] Meanwhile, in *CyberSource Corp. v. Retail Decisions, Inc.*, the method of using the internet to verify credit card actions was found to be unpatentable because the function of the internet was unnecessary to achieve the claim's objective.[69] Instead of actually performing a transformation, the internet acted as a data collector.[70] The Federal Circuit found this function insufficient to deem the internet necessary to the claim.[71]

The breadth of a claim is an additional factor—expansive coverage weighs against the claim's patentability because courts want to prevent claims "that too broadly preempt the use of a natural law."[72] The patent

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[64] *Benson,* 409 U.S. at 67.
[65] *See* SiRF Tech., Inc. v. Int'l Trade Comm'n, 601 F.3d 1319, 1333 (Fed. Cir. 2010).
[66] *See* Research Corp. Techs., Inc. v. Microsoft Corp.*,* 627 F.3d 859, 868 (Fed. Cir. 2010).
[67] *Id.*
[68] *SiRF*, 601 F.3d at 1333.
[69] CyberSource Corp. v. Retail Decisions, Inc., 654 F.3d 1366, 1375 (Fed. Cir. 2011).
[70] *Id.*
[71] *Id.*
[72] Mayo Collaborative Servs. v. Prometheus Labs., Inc., 132 S. Ct. 1289, 1294 (2012).

system was intended to foster and not foreclose innovation.[73] Since all inventions at some level utilize abstract ideas and natural law, innovation is "preempted" when a patent *disproportionately* ties up the use of underlying abstract ideas.[74] The Supreme Court has "repeatedly emphasized . . . patent law [must] not inhibit further discovery by improperly tying up the future use of laws of nature."[75] Because broader claims preempt more ideas than narrow claims, courts are more likely to find that they cover abstract ideas necessary for innovation.

The patentability of computer-implemented processes is a hotly contested issue with little certainty as to what constitutes patentable subject matter. Hoping to clarify the governing law, the Federal Circuit granted a petition for rehearing en banc in *CLS Bank International v. Alice Corp.*, requesting briefing on the appropriate test to determine "whether a computer-implemented invention is a patent ineligible 'abstract idea,'" and when, if ever, "the presence of a computer in a claim lend[s] patent eligibility to an otherwise patent-ineligible idea."[76] In *Alice*, the patent-in-suit claimed a computer trading platform for exchanging obligations in which a trusted third party settled obligations between a first and second party so as to eliminate "settlement risk."[77]

Despite the Federal Circuit's desire to bring consistency to the law, the *Alice* decision seemed to reflect the difficulty of the question of determining patentable subject matter. It contained "seven separate opinions reflecting at least three distinct approaches," with no single opinion garnering more than five judges' support.[78] The plurality opinion in *Alice* determined that the method claim did not cover patent-eligible material because there was "nothing in the asserted method claims that represent[ed] 'significantly more' than the underlying abstract idea for purposes of § 101."[79] Judge Lourie, writing for the plurality, stated that "[u]nless the claims require a computer to perform operations that are not merely accelerated calculations, a computer does not itself confer patent

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[73] *See* Graham v. John Deere Co., 383 U.S. 1, 6 (1966) (addressing the "constitutional command" that the patent system "must 'promote the Progress of . . . useful Arts'" (quoting U.S. CONST. art I, § 8, cl. 8)).
[74] *Prometheus*, 132 S. Ct. at 1294.
[75] *Id.* at 1301.
[76] CLS Bank Int'l v. Alice Corp. Pty. Ltd., 484 F. App'x 559, 559 (Fed. Cir. 2012) (granting request for rehearing en banc).
[77] CLS Bank Int'l v. Alice Corp. Pty. Ltd., 717 F.3d 1269, 1284–85 (Fed. Cir. 2013).
[78] Bernard Chao, *Interpreting* CLS Bank Int'l v. Alice, PATENTLY-O BLOG (Sept. 3, 2013, 3:08 PM), http://www.patentlyo.com/patent/2013/09/interpreting-cls-bank-intl-v-alice.html.
[79] *Alice*, 717 F.3d at 1287.

eligibility."[80] Judge Rader, however, noted that "nothing" in the *CLS Bank Int'l* decision "beyond [the] judgment has the weight of precedent."[81]

B. The Effect of Federal Circuit and Supreme Court Decisions on Virtual Compounds

For purposes of determining whether virtual compounds are patentable subject matter, it is helpful to analyze a sample claim. Since most of the claims contested in major § 101 decisions have been process claims, this analysis will utilize a sample process claim. However, patent eligibility does not depend merely on the form of the claim but instead on whether the claim's "inventive concept" amounts to something significantly more than an abstract idea or natural law.[82] Consider the following process claim from U.S. Patent No 6,083,711:

> 1. A method of identifying a candidate inhibitor compound capable of binding to, and inhibiting the proteolytic activity of, an alpha, or beta herpes protease, said method comprising:
> a) introducing into a computer program information derived from atomic coordinate defining an active site conformation of a herpes protease molecule based upon three-dimensional structure determination comprising a catalytically active site formed by at least the interaction of three amino acids Serine, Histidine and Histidine, wherein said program utilizes or displays the three-dimensional structure thereof;
> b) generating a three dimensional representation of the active site cavity of said protease in said computer program;
> c) superimposing a model of the inhibitor test compound on the model of said active site of said protease;
> d) assessing whether said test compound model fits spatially into the active site of said protease . . . .[83]

This claim can be broken down into simpler terms. The first step in the claim requires entering the virtual compound's coordinates into a computer program. The second step utilizes the computer to transform the coordinates into a three-dimensional structure. The third step requires the computer to superimpose a model of the test compound onto the active site of the virtual compound. The fourth step requires an assessment of the fit of the two compounds.

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[80] *Id*. at 1286.
[81] *Id*. at 1292 n.1.
[82] *See supra* notes 48–52 and accompanying text.
[83] U.S. Patent No 6,083,711 cols. 61–66 l. 25–51 (filed May 9, 1997). The patentees claimed a method for using their previously patented herpes protease compound in computer-aided drug design of possible herpes protease inhibitors.

Upon first glance, the immediate concern about the claim is that it only mentions a computer program, without specific mention of a machine. However, this concern need not affect the analysis of the claim; patent eligibility does not "depend simply on the draftsman's art."[84] Logically, the use of a computer program necessitates the use of a computer. While claims are not patentable simply because of computer implementation, they may be deserving of patent protection if they apply an abstract idea to a known structure or process in a way that demonstrates an "inventive concept."[85]

It remains to be determined whether this claim is directed to an abstract idea. One argument that it is might take the following form: The "inventive concept" is embodied in step four (part d) of the sample claim, which merely looks at two structures and inspects whether they fit. This is an abstract idea because the ability to determine fit is a mental process. The other two steps merely add a "generic computer function to facilitate performance" that is not enough to satisfy § 101.[86] Accordingly, just like the claim in *Alice*, the sample claim's use of a computer merely accelerates calculations.[87]

However, this simplification fails to recognize two other inventive concepts: the virtualization of a specific man-made compound by its atomic coordinates, and the utilization of a computer to produce a three-dimensional structure created from the coordinates. Step two of the claimed process involves the generation of a three-dimensional structure from atomic coordinates. It is infeasible for the human mind to superimpose a virtual test compound onto an active site of the virtual compound for purposes of determining its fit.[88] Unlike the method claimed in *Alice*, a human could not feasibly perform the task. In fact, most computers have trouble performing the necessary calculations because "the computational resources required to obtain exact . . . solutions . . . on a conventional computer generally increase exponentially with the number of atoms

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[84] Mayo Collaborative Servs. v. Prometheus Labs., Inc., 132 S. Ct. 1289, 1294 (2012) (quoting Parker v. Flook, 437 U.S. 584, 593 (1978)).
[85] *See supra* notes 48–52 and accompanying text.
[86] CLS Bank Intern. v. Alice Corp., 717 F.3d 1269, 1287 (Fed. Cir. 2013).
[87] *See id.*
[88] *See* SCOTT E. UMBAUGH, COMPUTER IMAGING, DIGITAL ANALYSIS AND PROCESS 5 (2005) (arguing that computer imaging is necessary when large database of data needs to be analyzed, because computer generated images enable humans to interpret this type of data).

involved."[89] The computer provides "the entire detailed 'solution,' without which it would be impossible to achieve the invention's purpose."[90]

The sample claim more closely resembles the claim from *Research Corp*. than the claim at issue in *Benson* and therefore should be patentable like the claim from *Research Corp*. In *Benson*, the claim covered a method of programming a general computer to convert binary-coded decimal numbers into pure binary through a mathematical algorithm.[91] Although the conversion of code in *Benson* might appear superficially similar to the conversion of atomic coordinate data into a virtual three dimensional image, the *Benson* claim involved inputs and outputs of a similar form—numbers converted into numbers. On the other hand, the conversion in this claim involves a form change from coordinates to spatial representation. It is simply not plausible that a human could mentally construct the spatial representation of a compound using its atomic coordinates.

While the machine-or-transformation test does not definitively prove the patentability of the sample claim,[92] the process's use of a computer supports the patentability of the claim. In *Alappat*, the Federal Circuit found that use of a specific program on a general-purpose computer makes the computer a specific machine.[93] Here, the sample claim is tied to a "specific machine" because the process claimed requires entering spatial coordinates into a specific computer program.[94] Any general computer lacking these specific programs would be incapable of performing the method.

Generating a three-dimensional representation of a compound from atomic coordinates is nearly impossible without that computer program. No other medium could generate the representation of the two compounds in a way that accurately could represent the compounds. Even with a computer, accurate portrayal of the compound is limited;[95] without the computer,

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[89] B.P. Lanyon, et. al., *Towards Quantum Chemistry on a Quantum Computer*, 2 NATURE CHEMISTRY 106, 106 (2010), *available at* http://arxiv.org/pdf/0905.0887.pdf.

[90] *See* CLS Bank Intern. v. Alice, 717 F.3d 1269, 1320 (Fed. Cir. 2013) (Moore, J., concurring in part and dissenting in part).

[91] Gottschalk v. Benson*,* 409 U.S. 63, 67 (1972).

[92] Bilski v. Kappos, 130 S. Ct. 3218, 3227 (2010) ("This Court's precedents establish that the machine-or-transformation test is a useful and important clue, an investigative tool, for determining whether some claimed inventions are processes under § 101. The machine-or-transformation test is not the sole test for deciding whether an invention is a patent-eligible 'process.'").

[93] *In re* Alappat, 33 F.3d 1526, 1545 (Fed. Cir. 1994).

[94] U.S. Patent No 6,083,711 cols. 61–66 l. 25–51 (filed May 9, 1997).

[95] *See* NAG & DEY, *supra* note 3, at 9 (observing that a lack of computing power has limited the use of computer-aided drug design).

effective portrayal would be impossible. The entire purpose of the claim is to use computer evaluation systems to quickly, easily, and cheaply examine compound inhibition of the virtual compound.[96] This purpose is thwarted without the use of the programmed computer. Just as the GPS receiver in *SiRF* was necessary to generate ranges to fulfill the goal of the claim,[97] the computer in the sample process is necessary to generate the three-dimensional structure required to fulfill the claim's purpose.

The narrow nature of the sample claim also favors patentability.[98] The Supreme Court has repeatedly warned against upholding patents that too broadly preempt a natural law. Virtual compound claims written like the sample claim preempt practically no natural law given the very limited use of one virtual compound in a computer system for purposes of computer-aided drug design. The sample claim would fail to preempt even an identical claim using different atomic coordinates because not "every limitation of the patent claim" would be identical.[99]

C. Patentability of Virtual Compounds and Patent Policy

By protecting virtual compounds, the patent system achieves its economic objectives.[100] The patent system prevents the inventor's compound from being used without authorization. As a result of the patentability of virtual compounds, the patent system entitles the inventor to a reward for her investment and sacrifice in developing the compound and ensures that others do not piggy back on that investment. Inventors are incentivized to continue developing drugs because the patent system gives them a monopoly over the compound in both physical and virtual form.

The patentability of virtual compounds also promotes the disclosure objective of the patent system. A researcher who discovered a promising target compound might refuse to reveal its formula, instead relying on trade secret law, if patent protection did not extend to cyberspace.[101] However,

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[96] U.S. Patent No 6,083,711 col. 26:61–65 (filed May 9, 1997) ("[U]sing these computer evaluation systems, a large number of compounds may be quickly and easily examined and expensive and lengthy biochemical testing avoided. Moreover, the need for actual synthesis of many compounds is effectively eliminated.").

[97] *See* SiRF Tech., Inc. v. Int'l Trade Comm'n, 601 F.3d 1319, 1333 (Fed. Cir. 2010).

[98] *See* Mayo Collaborative Servs. v. Prometheus Labs., Inc., 132 S. Ct. 1289, 1294 (2012) (citing O'Reilly v. Morse, 56 U.S. 62, 112–120 (1854)).

[99] Tate Access Floors, Inc. v. Maxcess Techs., Inc., 222 F.3d 958, 964 (Fed. Cir. 2000).

[100] *See* Field, *supra* note 23, at 1019–23 (discussing the underlying policies of patent law and how cyberspace protection of chemical compounds suits them).

[101] Admittedly, the value of today's pharmaceutical patents makes it unlikely that a researcher would refuse to patent the compound even if lacking virtual compound

with appropriate coverage in both concrete and virtual form, the researcher will be able to disclose the invention without losing his exclusive rights granted by the patent system.

CONCLUSION

Under current patent law, a patented compound would not be infringed by the use of the same compound in virtual form. However, specifically claiming the compound in virtual form would ensure protection from virtual infringement and would pass the § 101 inquiry due to the integral nature of the computer, the impossibility of executing the process mentally, and the narrow nature of a virtual compound claim. The patentability of virtual compounds achieves fairness for the inventor and the public in accordance with patent policy objectives.

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protection. However, without virtual compound protection, future advances in computer technology may decrease researcher's desire to disclose for a patent of the compound in physical form due the possible ease of using the compound in virtual form to create more effective drugs.