



(51) International Patent Classification:

G06F 19/16 (2011.01) G01N 33/68 (2006.01)
C40B 30/02 (2006.01) G06F 19/10 (2011.01)
G01N 33/53 (2006.01)

(21) International Application Number:

PCT/CA2015/000296

(22) International Filing Date:

5 May 2015 (05.05.2015)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

61/988,510 5 May 2014 (05.05.2014) US

(71) Applicant: CHEMATRIA INC. [CA/CA]; Suite 411, 112
College Street, Toronto, ON M5G 1L6 (CA).

(72) Inventors: HEIFETS, Abraham Samuel; 763 Spadina
Avenue, #204, Toronto, ON M5S 2J6 (CA). WALLACH,
Izhar; 990 rue Summerlea, Lachine QC H8T 2L6 (CA).
DZAMBA, Michael; 31 Elmwood Avenue North, Mis-
sissauga, ON L5G 3K1 (CA).

(74) Agent: NORTON ROSE FULBRIGHT CANADA LLP;
1 Place Ville Marie, Suite 2500, Montreal, Quebec H3B
1R1 (CA).

(81) Designated States (unless otherwise indicated, for every
kind of national protection available): AE, AG, AL, AM,
AO, AT, AU, AZ, BA, BB, BG, BH, BN, BR, BW, BY,
BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DK, DM,
DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT,
HN, HR, HU, ID, IL, IN, IR, IS, JP, KE, KG, KN, KP, KR,
KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG,
MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM,
PA, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, SA, SC,
SD, SE, SG, SK, SL, SM, ST, SV, SY, TH, TJ, TM, TN,
TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every
kind of regional protection available): ARIPO (BW, GH,
GM, KE, LR, LS, MW, MZ, NA, RW, SD, SL, ST, SZ,
TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, RU,
TJ, TM), European (AL, AT, BE, BG, CH, CY, CZ, DE,
DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU,
LV, MC, MK, MT, NL, NO, PL, PT, RO, RS, SE, SI, SK,
SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
GW, KM, ML, MR, NE, SN, TD, TG).

Published:

— with international search report (Art. 21(3))

(54) Title: BINDING AFFINITY PREDICTION SYSTEM AND METHOD

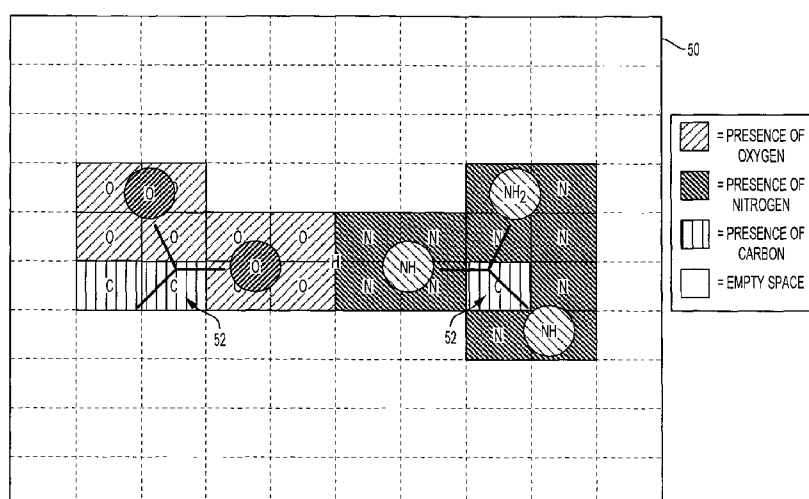


FIG. 5

(57) Abstract: Systems, devices, and methods for predicting binding affinity are disclosed. Records reflecting input data are stored. A data structure providing a geometric representation of binding input features is constructed. The data structure is populated by encoding data relating to at least one molecule and at least one target protein, the data for encoding selected from the stored input data. A predictive model is applied to the data structure to generate an indicator of a binding affinity for at least one molecule to at least one target protein.