

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property
Organization
International Bureau

(43) International Publication Date
24 July 2025 (24.07.2025)



(10) International Publication Number
WO 2025/155244 A1

(51) International Patent Classification:

G16B 15/30 (2019.01) G16C 20/50 (2019.01)
G16B 40/00 (2019.01) G16C 20/70 (2019.01)

(21) International Application Number:

PCT/SG2025/050009

(22) International Filing Date:

07 January 2025 (07.01.2025)

(25) Filing Language:

English

(26) Publication Language:

English

(30) Priority Data:

10202400124Q 16 January 2024 (16.01.2024) SG

(71) Applicant: **NANYANG TECHNOLOGICAL UNIVERSITY** [SG/SG]; 50 Nanyang Avenue, Singapore 639798 (SG).

(72) Inventors: **KONG, Wai-Kin Adams**; c/o Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798 (SG). **YIN, Yueming**; c/o Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798 (SG). **MU, Yuguang**; c/o Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798 (SG). **LI, Hoi Yeung**; c/o Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798 (SG).

(74) Agent: **VIERING, JENTSCHURA & PARTNER LLP**; 230 Victoria Street, #07-06 Bugis Junction Towers, Singapore 188024 (SG).

(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, CV, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IQ, IR, IS, IT, JM, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, MG, MK, MN, MU, 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, ST, SV, SY, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UY, UZ, VC, VN, WS, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, CV, GH, GM, KE, LR, LS, MW, MZ, NA, RW, SC, 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, ME, 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).

(54) Title: A SYSTEM AND METHOD FOR DETERMINING A BIOACTIVITY PARAMETER FOR A LIGAND

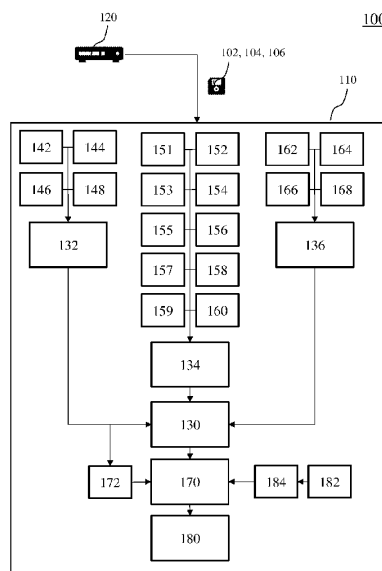


FIG. 1

(57) Abstract: Disclosed is a system and method for determining, a bioactivity parameter for a ligand, when the ligand is bound to a protein to form a ligand-protein complex, in a plurality of docking poses, comprising a processor configured to: obtain, ligand-protein complex structural data and reference bioactivity data; determine, a ligand-protein complex interaction parameter indicative of intermolecular interaction data of the ligand-protein complex in a docking pose; determine, an aggregated ligand-protein complex interaction parameter in the plurality of docking poses; and determine, the bioactivity parameter based on the aggregated ligand-protein complex interaction parameter, wherein determining the ligand-protein complex interaction parameter comprises, determining, a non-covalent parameter indicative of intermolecular interaction data of a ligand node and a protein node, based on, the ligand and protein attributes and a ligand-protein non-covalent parameter indicative of a binding stability of a type of dispersion force of the first non-covalent edge.

[Continued on next page]

Published:

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