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

(19) World Intellectual Property Organization
International Bureau

(43) International Publication Date
12 September 2025 (12.09.2025)

WIPO | PCT

(10) International Publication Number
WO 2025/188250 A1

(51) International Patent Classification:
G01N 27/62 (2021.01) *G16C 20/20* (2019.01)
G16C 20/70 (2019.01) *G16B 15/00* (2019.01)

(21) International Application Number:
PCT/SG2025/050164

(22) International Filing Date:
10 March 2025 (10.03.2025)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
10202400652R 08 March 2024 (08.03.2024) SG

(71) Applicant: **AGENCY FOR SCIENCE, TECHNOLOGY AND RESEARCH** [SG/SG]; 1 Fusionopolis Way, #20-10, Connexis North, Singapore 138632 (SG).

(72) Inventors: **TAY, Dillon Wei Peng**; c/o Institute of Sustainability for Chemicals, Energy and Environment, 1 Pesek Rd, Singapore 627833 (SG). **ANG, Shi Jun**; c/o Institute of High Performance Computing, 1 Fusionopolis Way, #16-16 Connexis, North Tower, Singapore 138632 (SG). **LIM, Yee Hwee**; c/o Institute of Sustainability for Chemicals, Energy and Environment, 1 Pesek Rd, Singapore 627833 (SG). **WONG, Zicong Marvin**; c/o Institute of High Performance Computing, 1 Fusionopolis Way, #16-16 Connexis, North Tower, Singapore 138632 (SG).

(74) Agent: **DAVIES COLLISON CAVE ASIA PTE. LTD.**; 10 Collyer Quay, #07-01 Ocean Financial Centre, Singapore 049315 (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,

(54) Title: COLLISION ENERGY SPECIFIC TANDEM MASS SPECTRAL PREDICTION

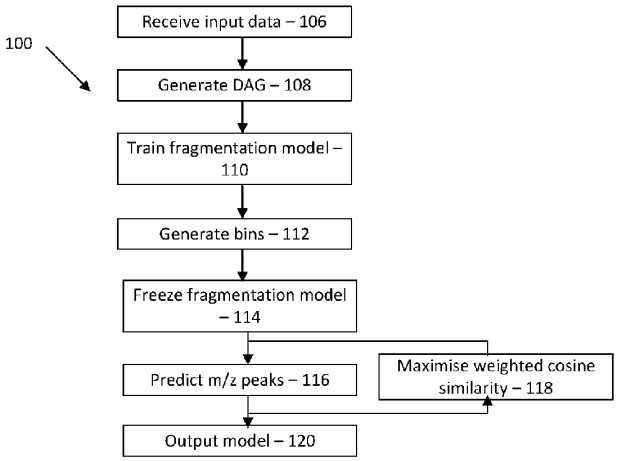


Figure 1B

(57) Abstract: A model is trained to predict collision-energy specific tandem mass spectra (MS/MS) for molecules. Directed acyclic graphs (DAG) are generated, that structurally relates predicted fragments for each molecule. A fragmentation model is then trained based on the DAGs and respective molecular inputs, to generate most probable fragments based on molecular inputs. The input data is then binned, with each bin corresponding to a non-overlapping collision energy range. The trained fragmentation model is frozen and intensity models (one for each bin) are trained to predict MS/MS spectra for molecules based on fragments generated by the fragmentation model.

[Continued on next page]

WO 2025/188250 A1

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).

Declarations under Rule 4.17:

— *of inventorship (Rule 4.17(iv))*

Published:

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

— *in black and white; the international application as filed contained color or greyscale and is available for download from PATENTSCOPE*