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| <p>(51) <b>International Patent Classification:</b><br/>G16C 20/30 (2019.01) G16C 60/00 (2019.01)<br/>G16C 20/70 (2019.01)</p> <p>(21) <b>International Application Number:</b><br/>PCT/US2024/016639</p> <p>(22) <b>International Filing Date:</b><br/>21 February 2024 (21.02.2024)</p> <p>(25) <b>Filing Language:</b> English</p> <p>(26) <b>Publication Language:</b> English</p> <p>(30) <b>Priority Data:</b><br/>18/114,398 27 February 2023 (27.02.2023) US</p> <p>(71) <b>Applicant:</b> DOW GLOBAL TECHNOLOGIES LLC<br/>[US/US]; 2211 H.H. Dow Way, Midland, Michigan 48674 (US).</p> <p>(72) <b>Inventors:</b> SCHMIDT, Alix; 2211 H.H. Dow Way, Midland, Michigan 48674 (US). CLARK, Ian; 2211 H.H. Dow Way, Midland, Michigan 48674 (US).</p> <p>(74) <b>Agent:</b> LORFING, Jason P.; Brooks, Cameron &amp; Huebsch, PLLC, 1201 Marquette Avenue S, Suite 400, Minneapolis, Minnesota 55403 (US).</p> | <p>(81) <b>Designated States</b> (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, UZ, VC, VN, WS, ZA, ZM, ZW.</p> <p>(84) <b>Designated States</b> (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).</p> |
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**(54) Title:** FORMULATION GRAPH FOR MACHINE LEARNING OF CHEMICAL PRODUCTS

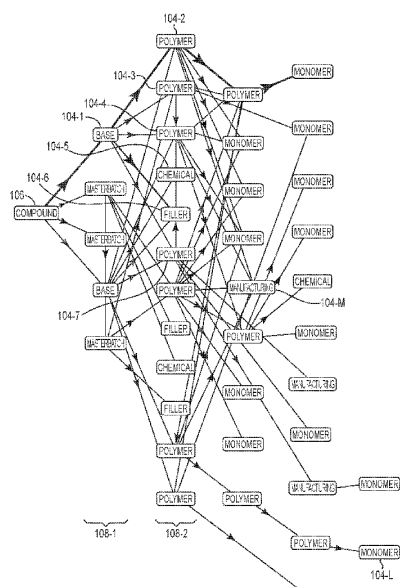


FIG. 1

**(57) Abstract:** Chemical formulations for chemical products can be represented by digital formulation graphs for use in machine learning models. The digital formulation graphs can be input to graph-based algorithms such as graph neural networks to produce a feature vector, which is a denser description of the chemical product than the digital formulation graph. The feature vector can be input to a supervised machine learning model to predict one or more attribute values of the chemical product that would be produced by the formulation without actually having to go through the production process. The feature vector can be input to an unsupervised machine learning model trained to compare chemical products based on feature vectors of the chemical products. The unsupervised machine learning model can recommend a substitute chemical product based on the comparison.

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