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(21) International Application Number: PCT/US99/09963 (22) International Filing Date: 7 May 1999 (07.05.99) (30) Priority Data: 09/073,845 7 May 1998 (07.05.98) US (71) Applicant: 3-DIMENSIONAL PHARMACEUTICALS, INC. [US/US]; Eagleview Corporate Center, Suite 104, 665 Stockton Drive, Exton, PA 19341 (US). (72) Inventors: AGRAFIOTIS, Dimitris, K.; 660 Perimeter Drive, Downingtown, PA 19335 (US). LOBANOV, Victor, S.; 24305 Cornerstone Drive, Yardley, PA 19067 (US). SALEMME, Francis, R.; 1970 Timber Lakes, Yardley, PA 19067 (US). (74) Agents: LEE, Michael, Q. et al.; Sterne, Kessler, Goldstein & Fox P.L.L.C., Suite 600, 1110 New York Avenue, N.W., Washington, DC 20005-3934 (US).		(81) Designated States: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, ARIPO patent (GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG). Published <i>With international search report.</i> <i>Before the expiration of the time limit for amending the claims and to be republished in the event of the receipt of amendments.</i>
(54) Title: SYSTEM, METHOD, AND COMPUTER PROGRAM PRODUCT FOR REPRESENTING PROXIMITY DATA IN A MULTI-DIMENSIONAL SPACE		
(57) Abstract <p>A system, method and computer program product for representing precise or imprecise measurements of similarity/dissimilarity (relationships) between objects as distances between points in a multi-dimensional space that represents the objects. Self-organizing principles are used to iteratively refine an initial (random or partially ordered) configuration of points using stochastic relationship/distance errors. The data can be complete or incomplete (i.e. some relationships between objects may not be known), exact or inexact (i.e. some or all of the relationships may be given in terms of allowed ranges or limits), symmetric or asymmetric (i.e. the relationship of object A to object B may not be the same as the relationship of B to A) and may contain systematic or stochastic errors. The relationships between objects may be derived directly from observation, measurement, a priori knowledge, or intuition, or may be determined indirectly using any suitable technique for deriving proximity (relationship) data. The present invention iteratively analyzes sub-sets of objects in order to represent them in a multi-dimensional space that represent the objects. In an exemplary embodiment, the present invention iteratively analyzes sub-sets of objects using conventional multi-dimensional scaling or non-linear mapping algorithms. In another exemplary embodiment, relationships are defined as pair-wise relationships or pair-wise similarities/dissimilarities between pairs of objects and the present invention iteratively analyzes a pair of objects at a time. Preferably, sub-sets are evaluated pair-wise, as a double-nested loop.</p>		