

(51) International Patent Classification:
G01N 21/35 (2006.01)(21) International Application Number:
PCT/US2011/050887(22) International Filing Date:
8 September 2011 (08.09.2011)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
12/880,903 13 September 2010 (13.09.2010) US(71) Applicant (for all designated States except US): **MKS INSTRUMENTS, INC.** [US/US]; 2 Tech Drive, Suite 201, Andover, MA 01810 (US).

(72) Inventors; and

(75) Inventors/Applicants (for US only): **TAN, Huwei** [US/US]; 706 Farms Drive, Burlington, MA 01803 (US). **WOLD, Svante, Bjarne** [US/US]; 42 Pine Hill Road, Hollis, NH 03049 (US).(74) Agent: **PICCOLOMINI, Zachary, P.**; Proskauer Rose, L.L.P., One International Place, Boston, MA 02110 (US).

(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, 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, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PE, PG, PH, PL, PT, QA, RO, RS, RU, RW, 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, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, 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, ML, MR, NE, SN, TD, TG).

Published:

- with international search report (Art. 21(3))
- with amended claims (Art. 19(1))

(54) Title: MONITORING, DETECTING AND QUANTIFYING CHEMICAL COMPOUNDS IN A GAS SAMPLE STREAM

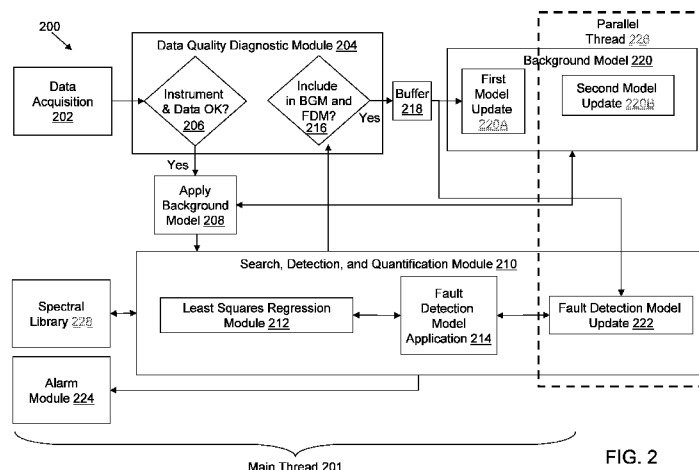


FIG. 2

(57) Abstract: Described are computer-based methods and apparatuses, including computer program products, for monitoring, detecting, and quantifying chemical compounds in a sample. A sample measurement comprising a digitized spectroscopic profile is received. A multivariate multistage background model comprising a first model that models a first time effect, a second model that models a second time effect that is different than the first time effect, or both is calculated. A background corrected sample measurement based on the sample measurement and the multivariate multistage background model is generated. A multivariate multistage library search, fault detection, and quantification algorithm is executed to identify one or more primary chemicals in the background corrected sample measurement. The search, detection, and quantification algorithm includes identifying one or more candidate chemicals in the background corrected sample measurement based on a multivariate statistical process control and identifying and quantifying a first primary chemical based on a focused chemical evaluation of the one or more candidate chemicals.