



(51) International Patent Classification:

G16C 20/20 (2019.01) H01J 49/00 (2006.01)

(21) International Application Number:

PCT/IB2021/057493

(22) International Filing Date:

13 August 2021 (13.08.2021)

(25) Filing Language:

English

(26) Publication Language:

English

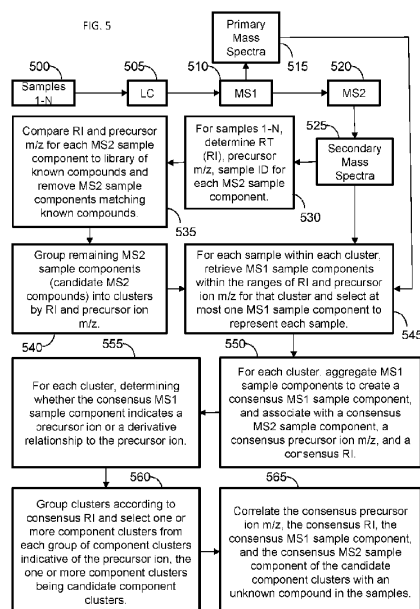
(30) Priority Data:

63/065,761 14 August 2020 (14.08.2020) US
63/116,239 20 November 2020 (20.11.2020) US(71) Applicant: **METABOLON, INC.** [US/US]; 617 Davis Drive, Suite 400, Durham, North Carolina 27560 (US).(72) Inventors: **DWYER, Rex A.**; 9504 Bells Valley Drive, Raleigh, North Carolina 27617 (US). **FREINKMAN, Elizaveta**; 102 Marble Falls Way, Cary, North Carolina 27519 (US). **EVANS, Anne M.**; 2801 Cameron Pond Drive, Cary, North Carolina 27519 (US).(74) Agent: **LYN, Kevin R.**; Womble Bond Dickinson (US) LLP, Attn: Patent Docketing, P.O. Box 7037, Atlanta, Georgia 30357-0037 (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, BN, BR, BW, BY, BZ, CA, CH, CL, CN, CO, CR, CU, CZ, DE, DJ, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IR, IS, IT, JO, JP, KE, KG, KH, KN, KP, KR, KW, KZ, LA, LC, LK, LR, LS, LU, LY, MA, MD, ME, MG, MK, MN, 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.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LR, LS, MW, MZ, NA, RW, 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, 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: METHOD FOR DETERMINING SMALL MOLECULE COMPONENTS OF A COMPLEX MIXTURE, AND ASSOCIATED APPARATUS AND COMPUTER PROGRAM PRODUCT



(57) Abstract: A data analysis method for a component separation / tandem mass spectrometer system, including first and second MS steps which data therefrom includes respective sample components (MS1-SC, MS2-SC), includes analyzing per sample a data set for MS2-SC to determine mass-to-charge ratio and retention index (m/z-RI) for each MS2-SC. m/z-RI for each MS2-SC is compared to a known compound library and matching MS2-SC removed from the data set, the remaining MS2-SC being candidate MS2-SC. Clusters are formed across the candidate MS2-SC, each having m/z-RI within respective ranges per cluster. For each sample within each cluster, MS1-SC within the cluster ranges are retrieved. For each cluster, at most one consensus MS1-SC represents each sample, with corresponding consensus MS2-SC and m/z-RI, and designated as a molecular ion or derivative thereof. Clusters are grouped by consensus RI and candidate clusters from each group are selected and correlated by consensus parameters with an unknown compound.

Declarations under Rule 4.17:

- *as to applicant's entitlement to apply for and be granted a patent (Rule 4.17(ii))*
- *as to the applicant's entitlement to claim the priority of the earlier application (Rule 4.17(iii))*

Published:

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