

Title (en)

METHOD FOR IDENTIFYING IN PARTICULAR UNKNOWN SUBSTANCES BY MASS SPECTROMETRY

Title (de)

VERFAHREN ZUR IDENTIFIZIERUNG INSBESONDERE UNBEKANNTER SUBSTANZEN DURCH MASSENSPEKTROMETRIE

Title (fr)

PROCÉDÉ D'IDENTIFICATION NOTAMMENT DE SUBSTANCES INCONNUES PAR SPECTROMÉTRIE DE MASSE

Publication

**EP 2389588 A1 20111130 (DE)**

Application

**EP 10707432 A 20100115**

Priority

- DE 2010000054 W 20100115
- DE 102009005845 A 20090121

Abstract (en)

[origin: CA2750231A1] The problem was to be able to use the mass spectrometrical analysis at the same time to determine the structure and/or families and/or the chemical properties of said substances, free of subjective evaluation, in the shortest amount of time, in an automatable fashion and with high accuracy, without requiring identical fragmentation patterns and/or defined comparison or identification rules. According to the invention, a fragmentation graph is formed from one or more mass spectrometrical fragmentation spectra of the substances, the data of the graph being compared to reference data preferably stored in an electronic database. The invention is used in particular in biological, pharmaceutical and chemical applications for determining the structure and/or the family and/or the chemical properties of unknown substances that are encountered.

IPC 8 full level

**G01N 33/68** (2006.01)

CPC (source: EP US)

**G01N 33/6848** (2013.01 - EP US); **Y10T 436/24** (2015.01 - EP US)

Designated contracting state (EPC)

AT BE BG CH CY CZ DE DK EE ES FI FR GB GR HR HU IE IS IT LI LT LU LV MC MK MT NL NO PL PT RO SE SI SK SM TR

DOCDB simple family (publication)

**DE 102009005845 A1 20100722**; CA 2750231 A1 20100729; EP 2389588 A1 20111130; JP 2012515902 A 20120712; JP 5559816 B2 20140723; US 2011278449 A1 20111117; US 8263931 B2 20120911; WO 2010083811 A1 20100729

DOCDB simple family (application)

**DE 102009005845 A 20090121**; CA 2750231 A 20100115; DE 2010000054 W 20100115; EP 10707432 A 20100115; JP 2011546588 A 20100115; US 201013145501 A 20100115