

Title (en)

A BINARY CODING METHOD FOR USE IN COMBINATORIAL CHEMISTRY

Title (de)

EINE BINÄRE KODIERUNGSMETHODE ZUR VERWENDUNG IN KOMBINATORISCHER CHEMIE

Title (fr)

PROCEDE DE CODAGE BINAIRE DESTINE A ETRE UTILISE EN CHIMIE COMBINATOIRE

Publication

**EP 0856067 A4 20050921 (EN)**

Application

**EP 96936686 A 19961018**

Priority

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- US 562395 P 19951019

Abstract (en)

[origin: WO9714814A1] The present invention is to a technique for labeling a ligand or compounds covalently bound to solid-phase-synthesis resin with a tag containing  $^{13}\text{C}$  and/or  $^{15}\text{N}$ . This tagging along with high-resolution isotope filtered  $^1\text{H}$  NMR, and Magic Angle Spinning probes provides for a technique which is general, nondestructive, and leaves the resin-bound sample intact and available for further chemical transformations. The limit of detection (< 800 pmol) in this system is sufficient to allow NMR to be used in deciphering the contents of a "one-bead, one-compound" combinatorial chemistry library.

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**G01N 24/08; C07B 61/00**

IPC 8 full level

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CPC (source: EP)

**C40B 50/16** (2013.01); **C40B 70/00** (2013.01); **B01J 2219/005** (2013.01); **B01J 2219/00572** (2013.01)

Citation (search report)

- [XY] G.C.LOOK: "Methods for combinatorial organic synthesis: The use of fast  $^{13}\text{C}$  NMR analysis for gel phase reaction monitoring", J.ORG.CHEM., vol. 59, no. 25, 1994, pages 7588 - 7590, XP002336433
- [Y] FITCH W L ET AL: "HIGH-RESOLUTION 1H NMR IN SOLID-PHASE ORGANIC SYNTHESIS", JOURNAL OF ORGANIC CHEMISTRY, AMERICAN CHEMICAL SOCIETY, EASTON, US, vol. 59, no. 26, 30 December 1994 (1994-12-30), pages 7955 - 7956, XP000974140, ISSN: 0022-3263
- [Y] K.L. WILLIAMSON ET AL: "Conformational analysis by nuclear magnetic resonance. Nitrogen-15 and carbon-13 spectra of lactams", J.AM.CHEM.SOC., vol. 98, no. 17, 1976, pages 5082 - 5086, XP002336434
- [PX] SARKAR, S.K. ET AL: "An NMR method to identify nondestructively chemical compounds bound to a single solid-phase-synthesis bead for combinatorial chemistry applications", J.AM.CHEM.SOC., vol. 118, no. 9, 6 March 1996 (1996-03-06), pages 2305 - 2306, XP002336089
- [PX] GEYSEN H M ET AL: "ISOTOPE OR MASS ENCODING OF COMBINATORIAL LIBRARIES", CHEMISTRY AND BIOLOGY, CURRENT BIOLOGY, LONDON, GB, vol. 3, no. 8, August 1996 (1996-08-01), pages 679 - 688, XP002035873, ISSN: 1074-5521
- [A] CHABALA J C ET AL: "BINARY ENCODED SMALL-MOLECULE LIBRARIES IN DRUG DISCOVERY AND OPTIMIZATION", PERSPECTIVES IN DRUG DISCOVERY AND DESIGN, ESCOM SCIENCE PUBLISHERS BV, vol. 2, 1994, pages 305 - 318, XP000654519, ISSN: 0928-2866
- [T] SHAPIRO M J ET AL: "NMR METHODS UTILIZED IN COMBINATORIAL CHEMISTRY RESEARCH", PROGRESS IN NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY, PERGAMON PRESS, OXFORD, GB, vol. 35, no. 2, 19 August 1999 (1999-08-19), pages 153 - 200, XP001183038, ISSN: 0079-6565
- See references of WO 9714814A1

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