

# Chemical Indexing as a Precision Tool for Relevant Patent Retrieval

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CAS Senior Product Manager  
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Fall 2011 ACS National Meeting



# CAS supports the mission of the ACS

## ACS Mission

To advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people.

## CAS Mission

To provide the world's best digital research environment to search, retrieve, analyze and link chemical information.



# CAS provides the world's most complete and authoritative coverage of chemistry and related science

## Substances

>61M organic and inorganic substances  
Updated daily (~12K)  
Substances reported in the literature back to 1802  
3 billion experimental and predicted properties

## Reactions

>35M single- and multi-step reactions  
>14M synthetic preparations  
Updated weekly (30K-50K)  
Reactions back to 1840

## CAS Content

## References

>34M patents, journals, dissertations, etc.  
>10K scientific journals covered  
Patents from 61 patent offices  
Updated daily (~4.5K)  
>290M citations back to 1997  
Coverage back to early 1800s

## Markush Structures

Markush structures representing organic and organometallic substances in patents  
Coverage back to 1961  
Updated daily (60-75 patent citations and 150-200 Markush structures)

# CAS has more than 100 years of experience analyzing and organizing disclosed chemistry from around the world



## US 824699 – First Indexed Patent

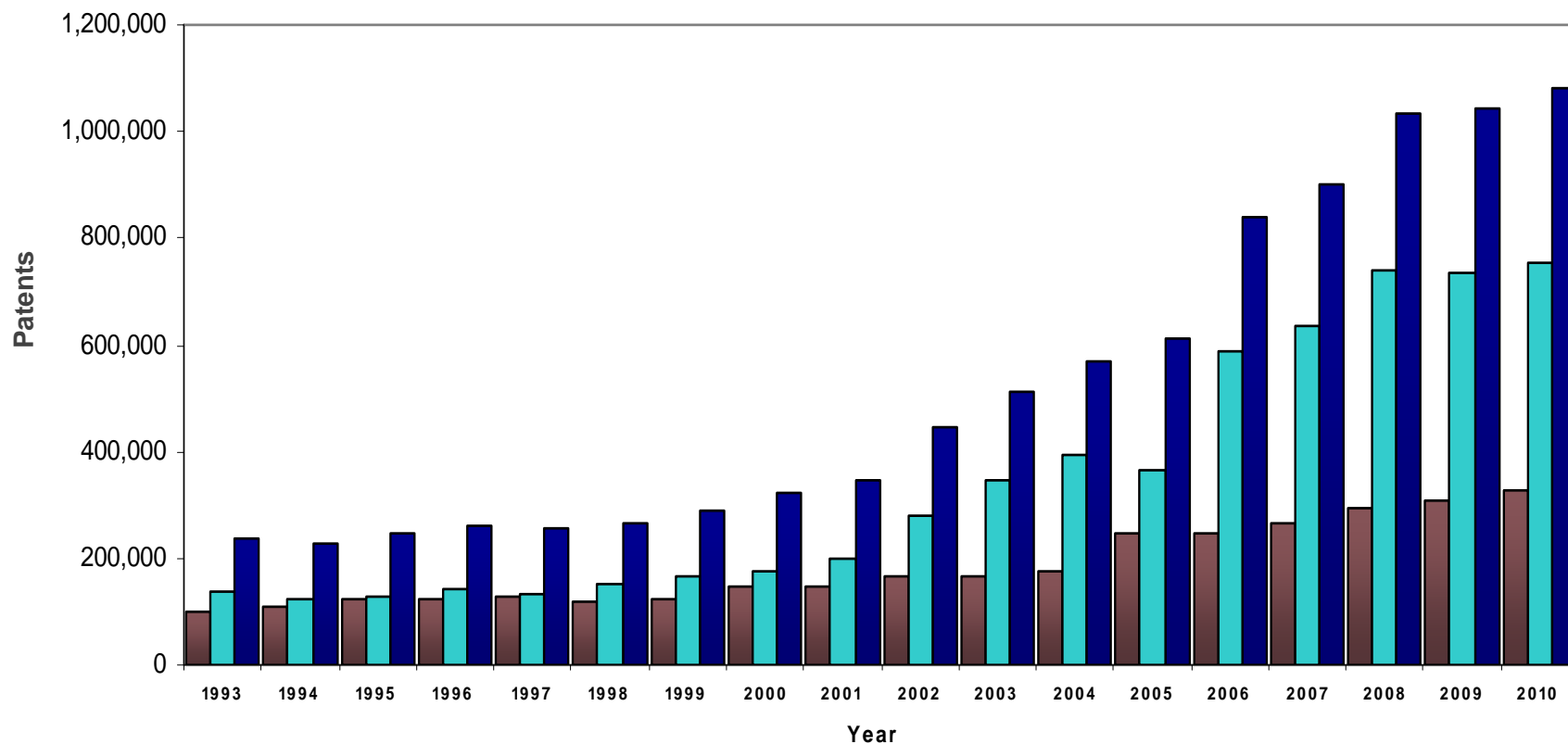


Patent coverage has expanded from 4,000 publications in 1907 to more than 1 million in 2010



# The number of patent publications CAS indexes continues to rise at a rapid pace

## Indexed Patent Documents in CAS Databases



■ Patent Indexed ■ Patent Equivalents ■ Total Patent Records

# CAS chemists select, abstract, index and enhance documents as they move through the editorial process

## Source Selection



## Document Indexing



## Reaction Indexing



## Markush Indexing



## Authority Process



## Patent selection helps make CAplus the most complete database of chemically related information


- CAplus covers 61 patent authorities
- Chemically related subject content is determined by IPCs assigned to the original patent
- Our website, [www.cas.org](http://www.cas.org), lists all covered patent classification codes



## CPlus ensures currency for major patent authorities

9 Major Patent Authorities (US, WO, EP, CA, DE, FR, GB, JP, RU)	• Within 2 days
1,500 "core" journals selected from more than 10,000 major scientific journals worldwide	• Within 7 days
Chinese, Korean and Indian Patent Offices	• Within 14 Days
Subject & Substance Indexing for major authorities	• Within 27 Days

# Indexing for major patent office documents is added quickly to the CPlus and CAS REGISTRY databases



US 20110054170A1

(19) **United States**  
 (12) **Patent Application Publication** (10) Pub. No.: **US 2011/0054170 A1**  
 McQuade et al. (43) Pub. Date: **Mar. 3, 2011**

(54) **SIX-MEMBERED N-HETEROCY CARBENE-BASED CATALYSTS ASYMMETRIC REACTIONS**

(75) Inventors: **D. Tyler McQuade**, (US); **Jin Kyoong Pa**, FL (US); **Matthew I Tallahassee**, FL (US); **Lackey, Hickory**, NC

(73) Assignee: **FLORIDA STATE RESEARCH FOUN**, TALLAHASSEE, FL

(21) Appl. No.: **12/870,901**

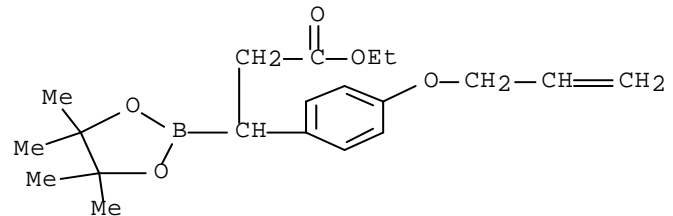
(22) Filed: **Aug. 30, 2010**

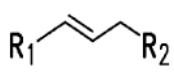
Related U.S. Application Data  
 (60) Provisional application No. 61/238,331, 2009.

ED **Entered STN: 04 Mar 2011**  
 AN 2011:271713 CAPLUS Full-text  
 DN 154:259821  
 TI Six-membered n-heterocyclic carbene-based catalysts for asymmetric reactions  
 IN McQuade, D. Tyler; Park, Jin Kyoong; Rexford, Matthew D.; Lackey, Hershel H.  
 PA Florida State University Research Foundation, USA  
 SO U.S. Pat. Appl. Publ., 22pp.  
 CODEN: USXXCO

DT  
 LA RN 1266612-72-9 REGISTRY  
 FAN. ED **Entered STN: 07 Mar 2011**  
 CN 1,3,2-Dioxaborolane-2-propanoic acid, 4,4,5,5-tetramethyl-.beta.-[4-(2-propen-1-yloxy)phenyl]-, ethyl ester (CA INDEX NAME)  
 MF C20 H29 B O5  
 SR CA  
 ● ●  
 LC STN Files: CA, CAPLUS, USPATFULL

PI  
 PRAI  
 ASSI  
 ● ●  
 IT





cis or trans

# The CAS indexing process enhances the retrieval and understanding of the original document

Patents, journals,  
web, catalogs, etc.

CAS

A division of the American Chemical Society

CAS Scientists



arXiv.org

Aldrichimica ACTA  
VOL. 46, NO. 1 • 2007

ACS  
chemical  
biology

Beilstein Journal of  
Organic Chemistry

division of polymer chemistry, inc  
American Chemical Society

J | A | C | S  
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ACS Chemical  
Neuroscience

THE JOURNAL OF  
PHYSICAL CHEMISTRY  
Letters

Cornell University  
Library

# CAS scientists use controlled vocabulary enhanced by natural language selected from the document

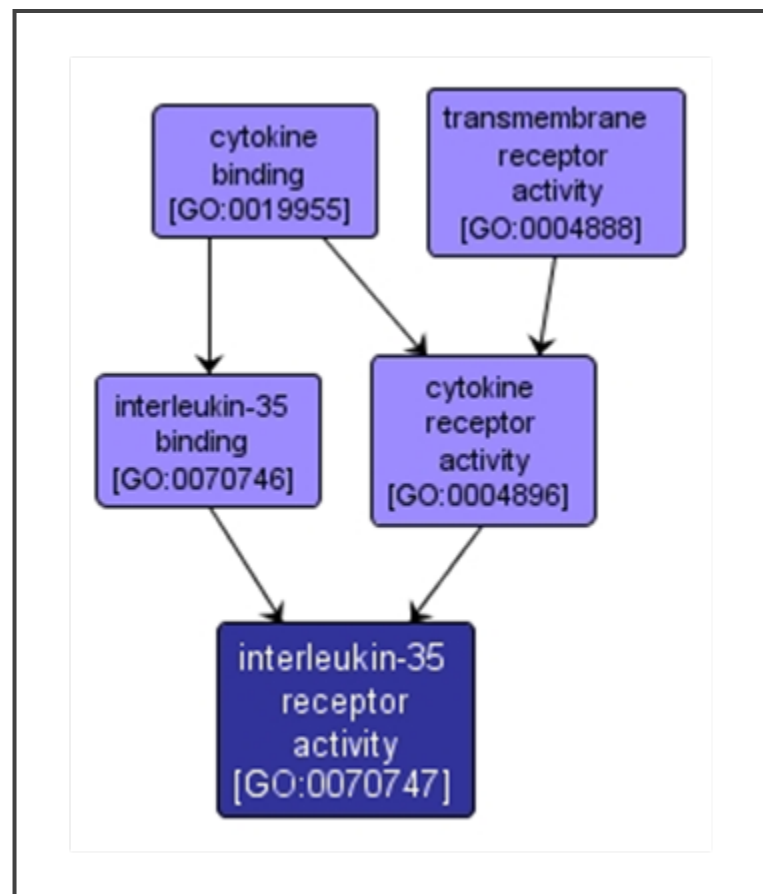
IT **Coating materials**  
(scratch-resistant; UV-curable acrylic hard coat transfer sheet with adhesive layer containing acrylic triblock copolymer)

IT **Antirheumatic agents**  
(disease-modifying, codrugs; preparation of thienopyrrole derivs. as cannabinoid receptor agonists useful in treatment and prevention of various disorders)

IT **Heterojunction semiconductor devices**  
**Nanowires**  
(Zn<sub>2</sub>TiO<sub>4</sub>-ZnO nanowire axial heterostructures formed by unilateral diffusion)

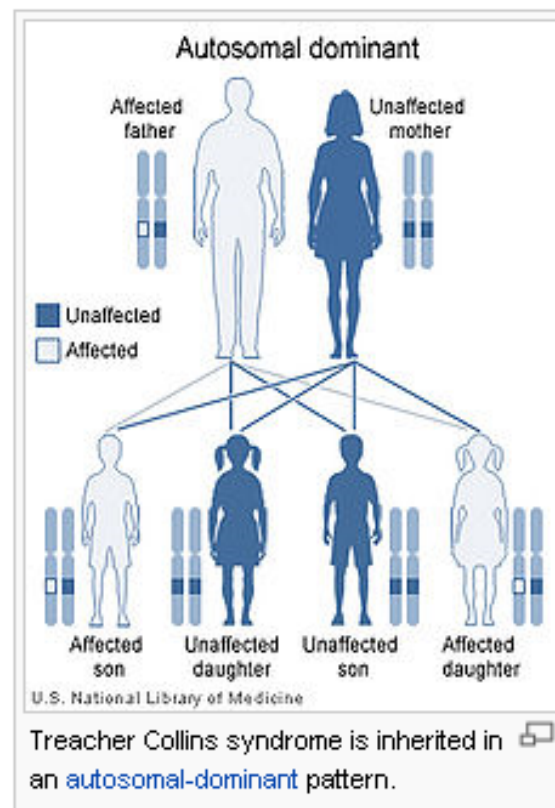
# Controlled vocabulary is constantly evolving because of new terminology in the source material...

- Frequently occurring terms
- New concepts that reflect the novelty reported
- Recent examples:
  - Albright-Goldman oxidation
  - Interleukin 35
  - PAT proteins



## ... and because of improved comprehension

- Monoclonal antibodies
  - OLD: Antibodies (L) monoclonal
- Controlled-release drug delivery systems
  - OLD: Drug delivery systems (L) controlled-release
- Treacher-Collins syndrome
  - OLD: Head and Neck, disease (L) Treacher Collins syndrome



## The CA Lexicon can be used to help focus a search

- General subject headings
- Chemical substance classes
- Taxonomic hierarchies

```
=> E CHROMATOGRAPHY+HIE/CT
E1      60903   BT1 Analysis/CT
E2      33301   BT1 Separation/CT
E3      123432  --> Chromatography/CT
E4      2335    NT1 Chromatographic stationary phases/CT
E5      774     NT2 Gas chromatographic stationary phases/CT
E6      382     NT3 Capillary gas chromatographic stationary
           phases/CT
E7      2530    NT2 Liquid chromatographic stationary phases/CT
E8      1172    NT3 Affinity chromatographic stationary phases/CT
E9      2803    NT3 HPLC stationary phases/CT
E10     715     NT4 Reversed phase HPLC stationary phases/CT
E11     174     NT3 Ion chromatographic stationary phases/CT
E12     303     NT2 Reversed phase chromatographic stationary phases/CT
```

# The CA Lexicon provides detailed taxonomic terminology arranged in a multi-level hierarchy

```

=> E PANAX+ALL/CT
E1          970      BT7  Organisms/CT
E2          8102     BT6  Eukaryota/CT
E3          14272    BT5  Plantae/CT
E4          1056     BT4  Magnoliophyta/CT
E5          1523     BT3  Magnoliopsida/CT
E6           11      BT2  Apiales/CT
E7          460      BT1  Araliaceae/CT
E8          970      BT3  Organisms/CT
E9          46205    BT2  Plants/CT
E10         3132     BT1  Medicinal plants/CT
E11         6390     -->  Panax/CT
                        HNTE Valid heading during volume 136 (2002)
                        to present.
                        NOTE Species of this genus are commonly known
                        as ginseng.
E12         2457     OLD  Ginseng/CT
E13         543      OLD  Ginseng (Panax)/CT
● ● ●
E31         288      NT1  Panax pseudoginseng/CT
E32          0      NT2  Panax pseudoginseng angustatus/CT
E33          1      NT2  Panax pseudoginseng elegantior/CT
E34          4      NT2  Panax pseudoginseng himalaicus/CT
E35          1      NT3  Panax pseudoginseng himalaicus
                        angustifolius/CT
E36          1      NT3  Panax pseudoginseng himalaicus
                        bipinnatifidus/CT
● ● ●

```

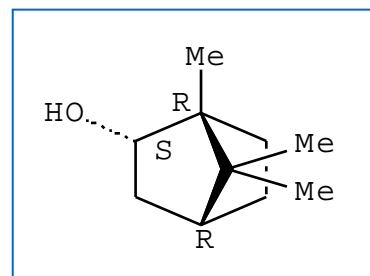
# Detailed indexing has been added to more than 50,000 Traditional Medicine patents

IT Analgesics  
 Ascites  
 Aspongopus  
 Astragalus  
 Atractylodes macrocephala  
 Aucklandia  
 Bupleurum  
 Cirrhosis  
 Edema  
 Epimedium  
 Fallopia japonica  
 Hepatitis  
 Ipomoea  
 Isatis  
 Ligusticum chuanxiong  
 Liver disease  
 Manis  
 Natural products, pharmaceutical  
 • • •  
 IT Abdominal disease  
     (abdominal distention)  
 IT Medical goods  
     (bags)  
 IT Viral hepatitis  
     (chronic)  
 • • •  
 IT 507-70-0  
     RL: BSU (Biological study  
     unclassified); BIOL (Biological study)

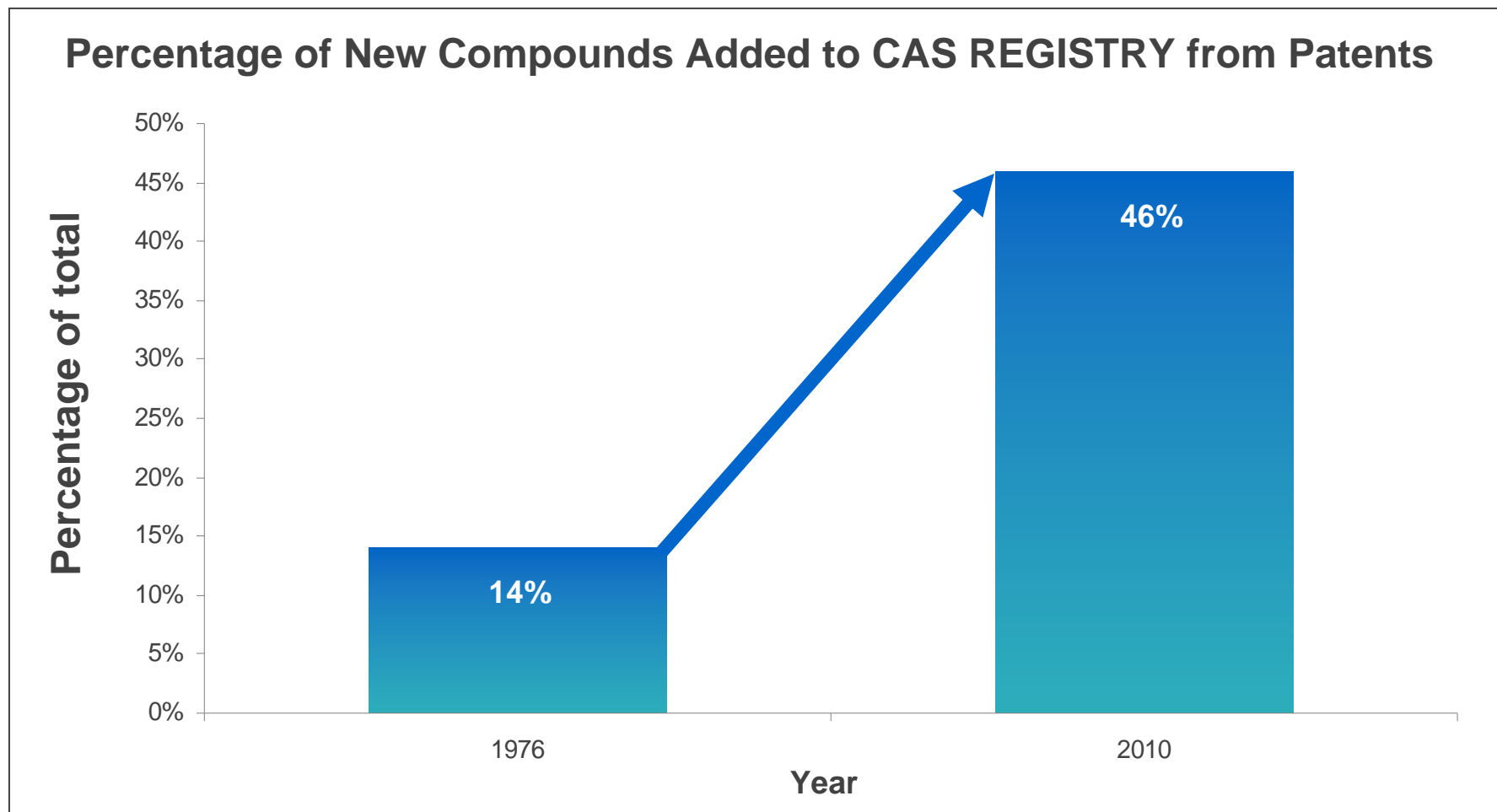
CA Indexing includes:

- Taxonomic terms
- Disease terms
- Substance class terms
- Specific substances

*Ligusticum chuanxiong* is one of the 50 fundamental herbs in traditional Chinese medicine.



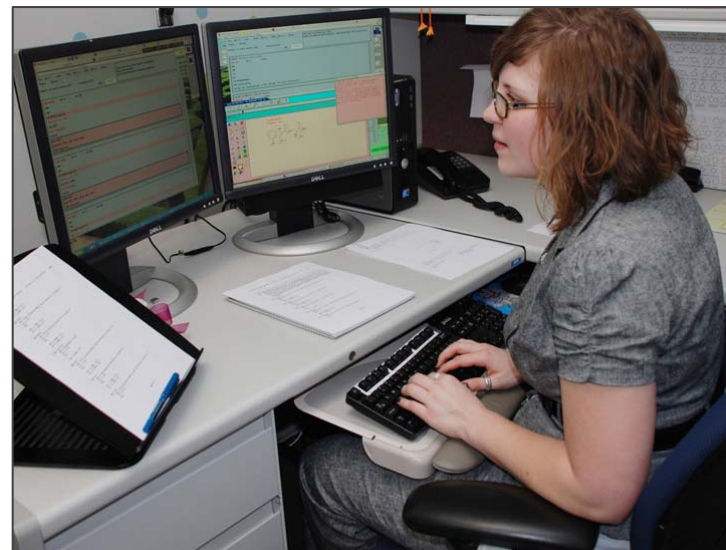
## Increasingly, new chemical discoveries are being disclosed through patent activities



# Substance indexing for CAS REGISTRY focuses on substances and their reported roles

## Indexers examine original documents for

- Substances reporting new or useful information
- Nomenclature, structures or additional chemical information
- Substance roles to be assigned



# Substance indexing for CAS REGISTRY focuses on substances and their reported roles

## Substance indexing for patents includes

- All specific substances from the claims
- Additional characterized substances from the description
- Uncharacterized substances from the Examples section, identified with Prophetic (PRPH) role
- Markush structures from both claims and disclosure that will appear in MARPAT




# Thousands of index entries are made for a typical patent publication


(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization  
International Bureau

(43) International Publication Date  
29 January 2009 (29.01.2009)



PCT



(10) International Publication Number  
**WO 2009/015208 A1**

(51) International Patent Classification:  
A01N 43/78 (2006.01) A61K 31/425 (2006.01)

(74) Agents: SWANSON & BRATTON  
8210 SouthPark Terrace, Littleton, CO 80120 (US)

(21) International Application Number:  
PCT/US2008/070893

(81) Designated States (unless otherwise indicated, all designated States except AU, AT, AU, AZ, BA, BB, BG, BI, BR, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, EG, ES, FI, GB, GD, GE, GH, GM, GN, GR, HK, IL, IN, IS, JP, KE, KG, KM, KN, KR, KZ, LA, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TD, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VE, VN, YU, ZA, ZM, ZW).

(22) International Filing Date: 23 July 2008 (23.07.2008)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:  
60/961,634 23 July 2007 (23.07.2007) US  
61/022,725 22 January 2008 (22.01.2008) US

(71) Applicant (for all designated States except US): REPLIDYNE, INC. [US/US]; 1450 Infinite Drive, Louisville, CO 80027 (US).

(84) Designated States (unless otherwise indicated, all designated States except AU, AT, AU, AZ, BA, BB, BG, BI, BR, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, EG, ES, FI, GB, GD, GE, GH, GM, GN, GR, HK, IL, IN, IS, JP, KE, KG, KM, KN, KR, KZ, LA, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PA, PE, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, ST, SV, SY, TD, TH, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VE, VN, YU, ZA, ZM, ZW).

(72) Inventors; and  
(75) Inventors/Applicants (for US only): GUILLES, Joseph [US/US]; 714 Skywalker Place, Lafayette, CO 80027 (US). JARVIS, Thule, Cross [US/US]; 2265 Dartmouth Ave., Boulder, CO 80305 (US). STRONG, Sarah [US/US]; 107 Lois SunDrive, Louisville, CO 80027 (US). SUN, Xicheng [US/US]; 1404 Kahler Place, Brown Field, CO 80027 (US). QIU, Jian [US/US]; 923 Grays Peak Drive, Superior, CO 80027 (US). ROHLOFF, John, C. [US/US]; 605 Meadowbrook Drive, Boulder, CO 80303 (US).

Published:  
— with international search report  
— before the expiration of the time claims and to be republished in amendments

## CAS analysis of a typical PCT application

- 917 indexed compounds from Examples and Claims
- 576 new compounds added to CAS REGISTRY
- 613 single-step reactions
- 5,394 multi-step reactions
- 1,029 reaction participants
- 2,119 substituent definitions for Markush structures added to MARPAT

# For complex chemistry, CAS chemists classify substance information and verify graphical processes and structures

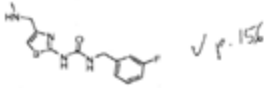
## 1. Review reaction and structure

WO 2006/015208 PCT/US2006/07993

Alternative process for Intermediate 4 Using Carbonyl Diimidazole:

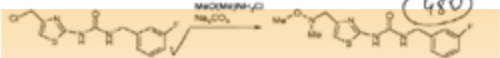
A stirred mixture of Intermediate 1: 2-amino-4-chloromethyl-thiazole hydrochloride (27.8 g, 0.15 mol), carbonyl diimidazole (25.5 g, 0.157 mol), and anhydrous THF (0.2 L) was treated dropwise with a solution of DIPEA (26.2 mL, 0.15 mol) in THF (20 mL) at 20-30 C. After 2-3 hours stirring, a solution of 3-fluorobenzylamine (18.5 mL, 0.164 mol) in THF (40 mL) was added. The reaction was diluted with water (200 mL) and THF was evaporated under reduced pressure. The residue was extracted with DCM (2 x 200 mL). The combined extracts were dried over sodium sulfate and concentrated to leave an orange resin that was purified by silica gel chromatography (acetone/hexane) to afford Intermediate 4 as a pale yellow solid (26 g, 58% yield). (1039)

Intermediate 5: 1-(3-Fluorobenzyl)-3-(4-(methylamino)methylthiazol-2-yl)urea

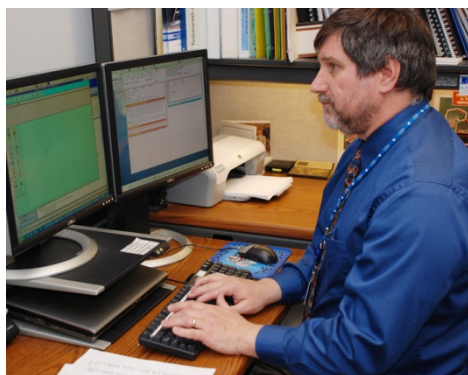


Prepared by reaction of Intermediate 4 with methylamine, following the procedure described for Intermediate 3. (1040)

Alternative Process for Intermediate 5 Using N,O-Dimethylhydroxylamine:



Step 1: 2-(3-(3-Fluorobenzyl)ureido)-4-(N-methoxy-N-methyl-amino)methylthiazole. A mixture of Intermediate 4, 2-(3-(3-Fluorobenzyl)ureido)-4-chloromethylthiazole (40 g, 0.133 mol), N,O-dimethylhydroxylamine (80 g, 0.820 mol), sodium carbonate (40 g, 0.754 mol), and abs. EtOH (0.2 L) was stirred and heated at 60-70 C for 8-12 hours. The mixture was diluted with water (0.8 L) and cooled to 20 C with continued stirring. The (480)



## 2. Create registration record

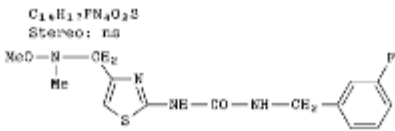
TAH	18772840Y	MUM	0480	Page	2681
ART	98-509999	WKU	81-227156-1480	2009-02-20	1108731-86-9 7
TD	012198564M	Chem	jkc56	01:49:47	Code 010 / M20050

INTD prepn. of antibacterial amide and sulfonamide substituted heterocyclic

Notes

MF C<sub>14</sub>H<sub>17</sub>FN<sub>4</sub>O<sub>2</sub>S

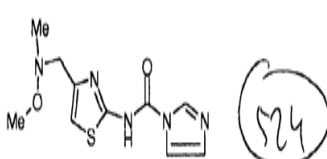
Chem



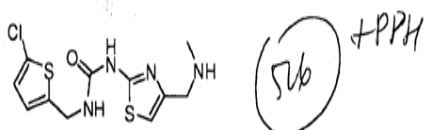
C<sub>14</sub>H<sub>17</sub>FN<sub>4</sub>O<sub>2</sub>S  
Stereo: NS

# CAS chemists interpret when compounds are described in terms other than singular structures or names

Intermediate 28: N-(4-((methoxy(methyl)amino)methyl)thiazol-2-yl)-1H-imidazole-1-carboxamide



Intermediate 29: 1-((5-Chlorothiophen-2-yl)methyl)-3-(4-((methylamino)methyl)thiazol-2-yl)urea



Step 1: Intermediate 28 (imidazole) was reacted with C-(5-chlorothiophen-2-yl)methylamine using Method 7. 1064

Step 2: The methoxyamino-urea product obtained in Step 1 was reduced with micronized 527 +PPH in acetic acid, following the procedure for Intermediate 5/Alternative Process/Step 2, to afford Intermediate 29.



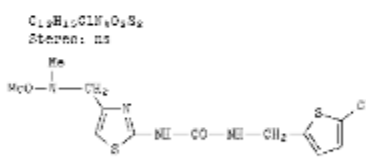
TAN 18772844Y	NUM 0527	Page 2714	
DAT 98-509999	W01 81-227156-1527	2009-02-20	1108712-44-2 T
TD 012198893M	Chem jku55	01:40:48	Code 010 / XD0050

human prope... of antibacterial... and sulfonamide substituted heterocycle

Name

MF C<sub>12</sub>H<sub>15</sub>ClN<sub>4</sub>O<sub>2</sub>S<sub>2</sub>

SM



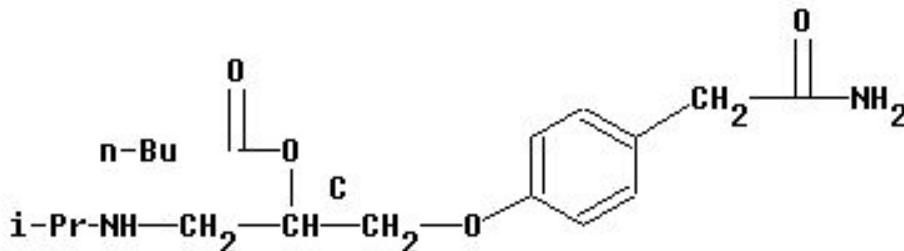
C<sub>12</sub>H<sub>15</sub>ClN<sub>4</sub>O<sub>2</sub>S<sub>2</sub>  
Stereo: ns

Methoxyamino-urea product

## CAS Registry Numbers allow precise targeting for specific substance searches

- Many names may be available for a substance
- Substance names may not be adequately descriptive
- Frequently no name is available
- A CAS Registry Number unambiguously identifies one unique substance

```
L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2011 ACS on STN
RN 1186034-68-3 REGISTRY
ED Entered STN: 22 Sep 2009
CN Pentanoic acid, 2-[4-(2-amino-2-oxoethyl)phenoxy]-1-
   [[(1-methylethyl)amino]methyl]ethyl ester (CA INDEX NAME)
OTHER NAMES:
CN Atenolol valerate
MF C19 H30 N2 O4
SR CA
LC STN Files: CA. CAPLUS
```



# CA Indexing for US20100331294 includes 75 additional uncharacterized substances from the examples

TABLE 2-continued

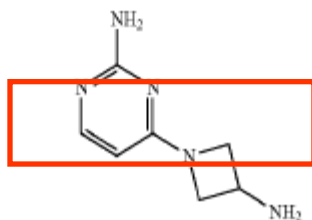
Examples 26-51.

May be Prepared by the Method of (substituting the indicated starting diamine)

Starting diamines  
Example (HNR<sup>1</sup>R<sup>2</sup>)  
Number and CAS#

Product Structures

31 tert-butyl azetidin-3-ylcarbamate  
CAS # 91188-13-5



Example 7A followed by Example 7B

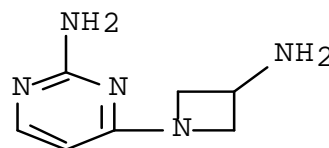
32 tert-butyl 2,7-diazaspiro[3.5]nonane-7-carboxylate  
CAS # 236406-55-6



Example 7A followed by Example 7B

33 tert-butyl 1,4-diazepane-1-carboxylate  
CAS # 112275-50-0

L1 ANSWER 21 OF 75 REGISTRY COPYRIGHT 2011 ACS on STN  
RN 1259941-53-1 REGISTRY  
ED Entered STN: 19 Jan 2011  
CN 2-Pyrimidinamine, 4-(3-amino-1-azetidiny)-  
(CA INDEX NAME)  
MF C7 H11 N5  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

IT	1201176-36-4P	1259941-43-9P	1259941-45-1P	1259941-47-3P
	1259941-50-8P	1259941-53-1P	1259941-56-4P	1259941-58-6P
	1259941-59-7P	1259941-63-3P	1259941-64-4P	1259941-66-6P
	1259941-68-8P	1259941-71-3P	1259941-73-5P	1259941-74-6P
	1259941-77-9P	1259941-79-1P	1259941-81-5P	1259941-82-6P
	1259941-85-9P	1259941-88-2P	1259941-89-3P	1259941-92-8P
	1259941-94-0P	1259941-96-2P		

RL: PAC (Pharmacological activity); PRPH (Prophetic); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of diaminopyrimidine derivs. as histamine H3 receptor ligands useful in treatment of diseases)

● ● ●

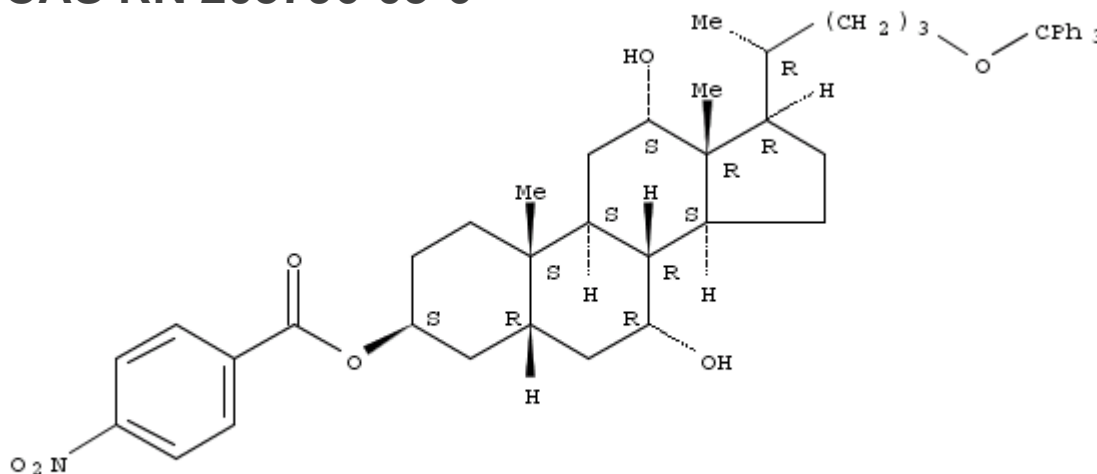
## Specific compounds are frequently not completely identified in the original document

Compound 34: Diisopropyl azodicarboxylate (DIAD) (1.20 mL, 6.08 mmol) was added to triphenylphosphine (1.60 g, 6.08 mmol) in THF (100 mL) at 0 °C. and was stirred for half an hour during which time the yellow solution became a paste.

Compound 14 (2.58 g, 4.06 mmol) and p-nitrobenzoic acid (0.81 g, 4.87 mmol) were dissolved in THF (50 mL) and added to the paste. The resulted mixture was stirred at ambient temperature overnight. Water (100 mL) was added and the mixture was made slightly basic by adding NaHCO<sub>3</sub> solution followed by extraction with EtOAc (3x50

mL). The combined extracts were washed with Na<sub>2</sub>SO<sub>4</sub>. The desired product (2.72 g) was purified by SiO<sub>2</sub> chromatography (Et<sub>2</sub>O/hexane 1:1) to give 2.72 g (40%) of the product. IR (neat): 2940, 2868, 1722, 1608, 1529, 1489, 1380, 1270, 1100, 8.30-8.26 (m, 2 H), 8.21-8.16 (m, 2 H), 7.80-7.75 (bs, 1 H), 4.02 (bs, 1 H), 3.90 (bs, 1 H), 3.80-3.75 (m, 1 H), 2.29-2.19 (m, 1 H), 2.07-1.95 (m, 1 H), 1.50-1.40 (d, J=6.6 Hz, 3 H), 0.70 (s, 3 H); <sup>13</sup>C NMR (CDCl<sub>3</sub>): 144.70, 136.79, 130.77, 128.88, 127.00, 126.00, 64.22, 47.79, 46.79, 42.15, 39.76, 37.00, 28.74, 27.71, 26.85, 26.30, 25.16, 23.00; MS (thioglycerol+Na<sup>+</sup> matrix) m/e: ([M+Na]<sup>+</sup>)

CAS RN 203796-03-6



Absolute stereochemistry.

# Indexing goes beyond the basic document to extract pertinent information out of the supplemental information

**JOC Article**  
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**Synthesis of the Sponge-Derived Plakortone Series of Bioactive Compounds**

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Received: June 22, 2010



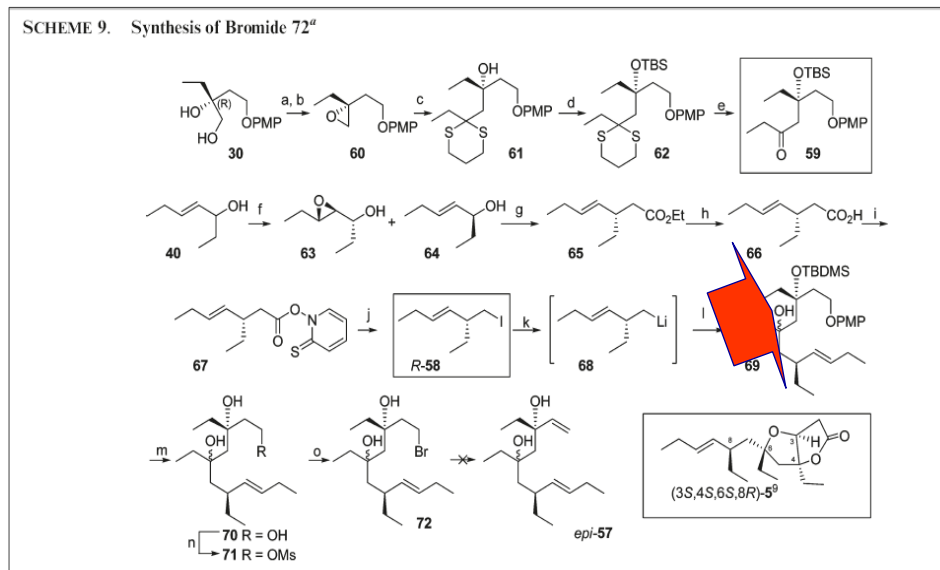
The Carcharias sponges of the genus *Plakortis*, *P. Achelradensis*, and *P. ampel* have provided a series of biologically active furanotriterpenes—the plakortones A–F (1–6) from the former sponge and B–F (7–11) from the latter. The defining motif of the plakortones is a uniquely composed 1,4-dioxane(2,3)-lactone–keto moiety, the emblematic furanotriterpene core. This core is efficiently accessed via a substituted Diels–Alder hydroacylation–hydroxylation–methylation cascade with an appropriate ened 1,3-diol. Total synthesis of plakortone C (3) and F (8) are now described which are constituting and emblematic features in this group of marine metabolites. Acylation of plakortone F (8) the most effective activator of ER- $\alpha$ —coupling ATPase, utilized novel diene derivatives that enabled from asymmetric dihydroxylation of ened 1,3-diol ened 20. A derived lactone moiety was then coupled with an independently generated, sulfonamide–methylolactone unit 21. The 1,2,3,4-tetraol motif gained through the subsequent treatment, stereoselective diol, was retained thereafter by stereoselective acylation via an efficient derivative. In this way, plakortone F (8) was demonstrated to possess the (1S,4S,6R,8R,11R) configuration. Marine plakortone F (8) was also accessed by using the Pd(II) induced sequence, but in this case, the required, complete acyclic diene was assembled from Plakortone C (3) instead from a sponges containing with (1R,2S,3S,4S)-2-methylpropylene, with a stereocenter 76. The diene primary alcohol 76 was converted by tandem-propenolone to key ened 80 which, with the Pd(II) sequence, afforded the majorly plakortone 80 and 81, with the former being identical with natural plakortone C (3). Very mild hydrogenation of 80 afforded a saturated plakortone, along with natural plakortone (8), that establishing its structure and absolute stereochemistry. Available information on the stereochemistry of plakortone F (8) and B (2) are also outlined so that the correct stereochemistry and absolute stereochemistry of plakortone B–F are now established.

**Keywords:** *Plakortone*; *Diels–Alder*; *hydroacylation*; *hydroxylation*; *methylation*; *Diels–Alder*; *hydroacylation*; *hydroxylation*; *methylation*; *Diels–Alder*; *hydroacylation*; *hydroxylation*; *methylation*

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**DOI:** 10.1021/jo101230q

**Publication:** *J. Org. Chem.* 2010, 75, 6689–6701. © 2010 American Chemical Society



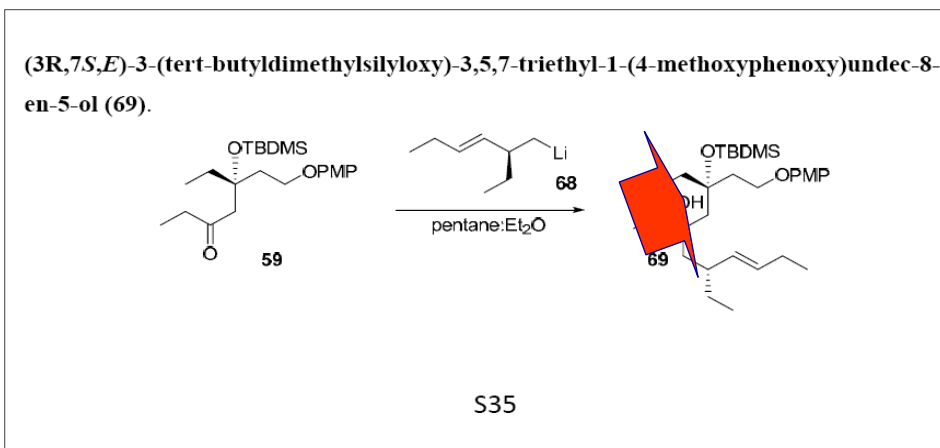
**Supporting Information**  
Synthesis of the Sponge-Derived Plakortone Series of Bioactive Compounds

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**Contents of Supporting Information**

The resonant CP-C14 side-chain and Wittig coupling including experimental data and NMR spectra for 100-107	S2 to S14
Synthesis of plakortone D (6)	S15 to S27
Synthesis of (2 <i>S</i> )-plakortone E (5)	S27 to S30
Synthesis of 72	S30 to S37
References	S38
Crystal data and ORTEP plot for the <i>p</i> -trinitrobenzene derivative of Compound 42	S39–S70

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L1          781 (NANOPARTICLE (S) SOLAR CELL)/B
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L2          886 (NANOPARTICLE (S) SOLAR CELL)/BI
=> S L2 NOT L1
L3          105 L2 NOT L1
AN          2009:79199  USPATFULL
TI          Solar cell and fabricating method thereof
IN          Chan, Chia-Hua, Taoyuan Hsien, TAIWAN, PROVINCE OF CHINA
            Chen, Chii-Chang, Taoyuan Hsien, TAIWAN, PROVINCE OF CHINA
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            Wu, Hung-Nan, Taoyuan Hsien, TAIWAN, PROVINCE OF CHINA
            Shing, Tai-Kang, Taoyuan Hsien, TAIWAN, PROVINCE OF CHINA
PA          National Central University (non-U.S. corporation)
PI          US 20090071532      A1  20090319
AI          US 2008-68218      A1  20080204 (12)
PRAI       TW 2007-96134166      20070913
DT          Utility
FS          APPLICATION
LREP       BIRCH STEWART KOLASCH & BIRCH, PO BOX 747, FALLS CHURCH, VA, 22040-
            0747, US
CLMN       Number of Claims: 19
ECL        Exemplary Claim: 1
DRWN       10 Drawing Page(s)
LN.CNT     379
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	PATENT	KIND	DATE
OS	CA 150:333965 *	US 20090071532	A1 20090319
* CA Indexing for this record included			
CC	52-2 (Electrochemical, Radiational, and Thermal		
ST	solar cell structure fabrication		
IT	Transparent materials		
	(adhesives, moisture-protection layer; structure and fabrication of solar cells with)		
IT	Microparticles		
	Nanoparticles		
	(antireflective layer; structure and fabrication of solar cells with)		
IT	Antireflective films		
	(microparticles and nanoparticles; structure and fabrication of solar cells with)		
IT	Polymers		
	(moisture-protection layer; structure and fabrication of solar cells with)		
IT	Micelles		
	(reverse; structure and fabrication of solar cells with)		
IT	Sol-gel processing		
	Solar cells		
	(structure and fabrication of solar cells)		
IT	Adhesives		
	(transparent, moisture-protection layer; structure and fabrication of solar cells with)		
IT	7631-86-9, Silica, uses	9003-53-6, Polystyrene	9011-14-7, Poly(methyl methacrylate)
	(microparticles and nanoparticles, antireflective layer; structure and fabrication of solar cells with)		

*nanoparticles* did not appear in close association with *solar cells* in this record

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