



### Subject Coverage

- Markush patents covered in CAplus<sup>SM</sup>
- Organo or organometallic molecules
- Polymers not included

### File Type

Markush Structure, Training

#### **Features**

Thesaurus None Alerts (SDIs) None CAS Registry Learning **SLART**  $\overline{\mathbf{V}}$  $\mathbf{\Lambda}$ Number<sup>®</sup> Database Identifiers Page Images Keep & Share Structures  $\overline{\mathbf{Q}}$  $\mathbf{\Lambda}$ 

### Record Content

- Markush structures found in the claims and often the disclosure of the patent, bibliographic information, patent family information, cited references
- In-depth substance and subject indexing including CAS Registry Numbers®, and an abstract, all of which are displayable
- The structures are searchable
- Document information can be searched in CA<sup>SM</sup> and CAplus

### File Size

569 records (02/16)

### Coverage

Selected Markush structure records for patents found in CAplus with the patent publication year of 1988-1989

### **Updates**

None

### Language

English

### **Database** Producer

Chemical Abstracts Service 2540 Olentangy River Road

P.O. Box 3012

Columbus, Ohio 43210-0012 USA Phone: 800-753-4227 (North America) Phone: 614-447-3700 (worldwide)

614-447-3751 Fax: Email: help@cas.org Copyright Holder

Sources	Selected Markush patents found in CAplus		
User Aids	<ul> <li>Online Helps (HELP DIRECTORY lists all help messages available)</li> <li>STNGUIDE</li> </ul>		
Clusters	LEARNING     STN Database Clusters Information		
Related Databases	MARPAT		
Pricing	Enter HELP COST at an arrow prompt (=>).		

### **SEARCH and DISPLAY Field Codes**

There are no fields that allow left truncation.

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from the textual information associated with the Markush structures) (1)	None (or /BI)	S MESO S PHARMACEUT? (L) SALT#	MSTR
Accession Number Entry Date (2) Update Date (2)	/AN /ED /UP	S 118:93622/AN S 19990305/ED S L1 AND UP>=19990100	AN Not displayed Not displayed

<sup>(1)</sup> Only structure-related text terms are included; terms from the CAplus Basic Index are not searchable.

### **Structure Search Terms**

Novice SEARCH provides prompts to allow you to modify some query attributes, e.g., MLEVEL, before search is run.

Term	Search Examples
L-number of a structure built using the STRUCTURE command or uploaded from STN Express (1)	SEARCH L1 CSS FUL S L2 S L7 SUBSET=L5

<sup>(1)</sup> The L-number answer set from a structure search may be combined with text terms, e.g., S L6 AND SALTS.

## **Types of Structure Searching**

Novice SEARCH provides prompts to allow you to modify some query attributes, e.g., MLEVEL, before the search is run.

Туре	Definition	Search Code	Search Examples
Substructure (default) Closed Substructure	Search for substances that match the query. Substitution is allowed at all open positions. Search for substances that match the query exactly. Substitution is allowed at positions opened by CONNECT.	SSS CSS	SEARCH L1 SSS FUL S L2 SEARCH L1 CSS FUL SEA L4 CSS SUB=L2

<sup>(2)</sup> Numeric search field that may be searched using numeric operators or ranges.

### **Scopes of Structure Searches**

Novice SEARCH provides prompts to allow you to modify some query attributes, e.g., MLEVEL, before the search is run.

To create an L-number answer set containing candidate structures that have passed the screening step of your structure search, enter EXTEND on the search command line or enter SET EXTEND ON or SET EXTEND ON PERM at an arrow prompt (=>). For details, enter HELP SET EXTEND at an arrow prompt.

Scope	Definition	Search Code	Search Examples
Sample (default)(1)	Search a fixed 5% of the file	SAM	SEARCH L1 SAM SSS
Full	Search 100% of the file	FUL	S L5 SSS FUL
Range	Search a user-specified portion of the file	RAN	S L4 RAN=(V117,)
Subset Sample	Search a fixed sample of an answer set created by a search in MARPAT	SUB SAM	S L7 CSS SUB=L5 SAM
Subset Range	Search a user-specified portion of an answer created by a search in MARPAT	SUB RAN RAN=(V118)	S L3 SUB=L2
Subset Full	Search 100% of an answer set created by a search in MARPAT	SUB FUL	S L8 SUB=L6 FUL

<sup>(1)</sup> EXTEND is not valid with SAMPLE.

### **DISPLAY Formats**

Any combination of formats may be used to display answers. Multiple codes must be separated by spaces or commas. The fields are displayed in the order requested, e.g., D TI AU. The PRINT command is not valid in MARPAT. The default Generic Group display (expanded form) has GTEXT set to ON. To use the compact form, enter SET GTEXT OFF at an arrow prompt (=>).

Hit-term highlighting is available in the AN and MSTR fields. MARHIGHLIGHT must be ON during SEARCH in order to use HIT, FHIT, FQHIT, and QHIT formats.

Format	Content	Examples
AB	Abstract Text	D AB
AI (AP) <b>(1)</b>	Patent Application Information	D AI PI
AI.B (AP.B) (1)	Patent Application Information, Basic	D AI.B
AN	Accession Number	DISPLAY L2 1-10 AN
		HIT
ANPL	AN and CAplus Accession Number	D ANPL
CC	CA Classification Code (CA section and section cross-references)	D CC
CT <b>(2)</b>	Controlled Term	D CT
CYA <b>(2)</b>	Country of Author	D CYA
CYC (CY.CNT) (2)	Patent Country Count	D CYC
DS (2)	Designated States	D PI DS
DS.B <b>(2)</b>	Designated States, Basic	D DS.B
DT (TC)	Document Type	D DT
FS <b>(2)</b>	File Segment (Section Group)	D FS
GI <b>(3)</b>	Graphic Image or Graphic Image Information	D GI
ICA	Additional or Supplementary IPC	D 2-10 ICA
ICI	Index or Complementary IPC	D 5 8 ICI
ICM	Main IPC	D ICM
ICS	Secondary IPC	D ICS
IN (AU)	Inventor Name	DIN
ISN (2)	International Standard (Document) Number	DISN
IT (4)	Index Term and CAS role	D AN IT
LA	Language	DLA
MSTR	All Markush structures and related text	D AN MSTR
MSTR(n) <b>(2)</b>	Markush structure n and its related text	D AN MSTR (1)
NCL	National Patent Classification	D NCL
OS	Other Source	DOS

**DISPLAY Formats (cont'd)** 

Format	Content	Examples
PA (CS)	Patent Assignee	D PA
PI <b>(1)</b>	Patent Information Table	D TI PI
PI.B (PN.B) <b>(1,2)</b>	Patent Information, Basic	D PI.B
PN	Patent Number	D PN
PNC (PN.CNT) (2)	Patent Number Count	D PNC
PNK	Patent Number Count  Patent Number/Kind Code	D PNK
PNK.B	Patent Number/Kind Code, Basic	D PNK.B
		D AI PRAI
PRAI (PRN) (1)	Priority Application Information Priority Application Information, Basic	D PRALB
PRAI.B (PRN.B)(1)	Publication Year	D PY
PY <b>(2)</b>		D TI PY.B
PY.B <b>(2)</b>	Publication Year, Basic Cited References	D TI RE
RE (3)		
RETABLE (2,3)	Cited References Table	D TI AU RETABLE
RE.CNT (REC) (3)	Citing Document's Reference Count	D REC
RL (4)	Index Term and CAS role	D RL
RN <b>(2)</b>	CAS Registry Numbers	D AN RN
SO	Source	D TI AU SO
ST	Supplementary Term (CA keyword)	D ST
SX <b>(2,5)</b>	CA Section Cross-Reference Code	D TI SX
TI	Title of Document	D TI MSTR
ABS	GI, AB	D ABS
ALL (1,4)	AN, TI, IN, PA, SO, DT, LA, NCL, CC, FAN.CNT, PI, PRAI, OS, GI,	D L2 1-7 ALL
, (.,.,	AB, ST, IT, RL, RE.CNT, RE, MSTR	D 22 1 7 7.22
APPS (1)	Al, PRAI	D APPS
APPS.B (1)	Al.B, PRAI.B	D APPS.B
BIB (1)	AN, TI, IN, PA, SO, DT, LA, FAN.CNT, PI, PRAI, OS, RE.CNT (BIB	D 1-3 BIB HIT
DID (1)	is the default)	D 1 0 BIB 1 11 1
CAN	List of CA Abstract Numbers (no L-number header)	D CAN
CBIB	AN, plus Compressed Bibliographic Data	DISPLAY L1 1 CBIB
DALL <b>(1,4)</b>	ALL, delimited for post-processing	D DALL
DMAX (1,4)	MAX, delimited for post-processing	D MAX
FAM <b>(1)</b>	AN, FAN.CNT, PI for the accession number, plus PI for other family	D FAM
i Aivi (i)	accession numbers	DIAW
FAN	Family Accession Number (AN, FAN.CNT, FAN)	D FAN
FBIB (1)	BIB plus PI for other family accession numbers	D FBIB
IABS	ABS, with text labels	D IABS
		D IALL
IALL (1,4)	ALL, indented with text labels	
IBIB <b>(1)</b>	BIB, indented with text labels	D IBIB
IC	International Patent Classification, Main and Secondary	D IC
IDE	AN, MSTR	D IDE
IMAX (1,4)	MAX, indented with text labels	D IMAX
IND <b>(4)</b>	IPC, NCL, CC, ST, IT, RL	D TI IND
IPC	International Patent Classifications (IC (ICM, ICS), ICA, ICI)	D IPC
ISTD (1)	STD, indented with text labels	D ISTD
MAX (1,4)	ALL, plus PI for other family accession numbers	D MAX
OBIB (1)	BIB, Original (AN, TI, IN, PA, SO, PI, DS, AI, PRAI, DT, LA, OS)	D OBIB
OIBIB (1)	OBIB, indented with text labels	D OIBIB
PATS (1)	SO, PI	D PATS
SAM <b>(4)</b>	IPC, NCL, CC, SX, TI, ST, IT, and FQHIT	DIS SAM 1-5
SBIB <b>(1)</b>	BIB, without RE.CNT (AN, DN, TI, AU, IN, CS, PA, SO, PB, DT, LA, FAN.CNT, PI, PRAI, OS)	D 1 3 SBIB
SCAN (3,4,6)	IPC, NCL, CC, TI, ST, IT, RL, FQHIT (random display, no answer	D SCAN
	numbers)	
SIBIB (1)	SBIB, indented with text labels	D SIBIB
	LANDEL IN DA CO DE LA FANCOIE DI DDALNIOL CO	
STD (1)	AN, TI, IN, PA, SO, DT, LA, FAN.CNT, PI, PRAI, NCL, OS, RE.CNT	D STD

**DISPLAY Formats (cont'd)** 

Format	Content	Examples
FHIT	The first full Markush structure that matches the query structure and (or) the fields containing hit text terms	D CBIB ABS FHIT
FQHIT (7,8)	Portions of the first Markush structure that match the query structure and (or) fields containing the first query focus hit text terms	D FQHIT
FQHITEXG (7,9)	FQHIT plus definitions for unmatched G-groups that are visible in the assembled display	D FQHITEXG
HIT	The full Markush structure(s) that match the query structure and (or) the fields containing hit text terms	D CBIB ABS HIT
QHIT (7,8)	The portions of each Markush structure that match the query structure and (or) the fields containing hit text terms	D QHIT
QHITEXG (7,9)	QHIT plus definitions for unmatched G-groups that are visible in the assembled display	D QHITEXG

- (1) By default, patent, application, and priority numbers are displayed in STN format. To display them in Derwent format, enter SET PATENT DERWENT at an arrow prompt. To reset display to STN format, enter SET PATENT STN.
- (2) Custom display only.
- (3) No online display fee for this format.
- (4) By default, roles are displayed as codes and text. To suppress the display of role codes and text, enter SET ROLES OFF. To display only codes, enter SET ROLES CODES.
- (5) SX displays all information in the CC field, i.e., CA section and section cross-references.
- (6) SCAN must be specified on the command line, i.e., D SCAN or DISPLAY SCAN.
- (7) SET MPTASSEMBLY command allows you to control answer assembly formats and is set ON as a system default. To change the MARPAT display, enter SET MPTASSEMBLY BOTH or SET MPTASSEMBLY OFF. If MPTASSEMBLY is set to BOTH or ON and assembly is not possible, only the unassembled display will be shown. For more information on SET MPTASSEMBLY see HELP T13 in MARPAT.
- (8) If you want to retain the original FQHIT/QHIT format, SET MPTASSEMBLY OFF.
- (9) Even if MPTASSEMBLY is set to OFF, the unmatched G-group definitions available in the QHITEXG and FQHITEXG formats will only be shown with assembled displays. If MPTASSEMBLY is set to BOTH, an unassembled display will follow.

### Displaying CAplus or MEDLINE documents for cited references

Enter the following in the DISPLAY command: L-number for the answer set; answer number (only one may be specified); RAN.CAPLUS(x-y), RAN.MED(x-y) where (x-y) is the cited reference number, numbers, or range of numbers; and the display format for the document to display, e.g., BIB ABS. For example, to display CAplus records for the cited references 1 and 2 from answer 2 in the answer set L5, enter the following:

=> D RAN.CAPLUS(1-2) L5 2 BIB ABS

### SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Field Name	Field Code	ANALYZE/ SELECT	SORT
Abstract Text	AB	Y	N
Accession Number	AN	Y (1)	N
Author (Inventor)	AU	Υ	Υ
CA Classification Code (section and subsection)	cc	Υ	Υ
CA Section Cross-Reference Code	SX	Υ	Υ
CAS Registry Number	RN	Y (2)	N
CAS Role	RL	Y	N
Cited References	RE	Υ	N
Cited Reference(n)	RE(n)	Y (3)	N

# SELECT, ANALYZE, and SORT Fields (cont'd)

Field Name	Field Code	ANALYZE/ SELECT	SORT
Cited Reference Accession Number in CAplus	RAN.CAPLUS	Y (4)	N
Cited Reference Accession Number(n) in CAplus	RAN.CAPLUS(n)	Y (3,4)	N
Cited Reference Accession Number in MEDLINE	RAN.MED	Y (5)	N
Cited Reference Accession Number(n) in MEDLINE	RAN.MED(n)	Y (3,5)	N
Cited Reference Author Name	RAU	Y	N
	RIN	Y (6)	N
Cited Reference Count	RE.CNT	Y	Υ
	REC	Y	Y
Cited Reference Patent Number	RPN	Υ	N
Cited Reference Publication Year	RPY	Υ	N
Cited Reference Work Title	RWK	Υ	N
CODEN	CODEN	Y (7)	Υ
Controlled Term	CT	Y	N
Corporate Source (Patent Assignee)	cs	Υ	Υ
Country Name of Author	CYA	Υ	Υ
Designated State	DS	Υ	N
Designated States, Basic	DS.B	Y (8)	N
Document Type	DT	Y	Υ
Family Accession Number	FAN	Ý (9)	N
File Segment	FS	Y	Y
Index Term	İT	Y	N N
International Standard (Document) Number	ISN	Ý (10)	N N
International Standard Serial Number	ISSN	Υ (1.5)	Y
Inventor Name	IN	Ý	Ϋ́
IPC	IPC	Ý (11)	Ϋ́
IPC, Additional or Supplementary	ICA	Y	Ý
IPC, Index or Complementary	ICI	Ý	Ϋ́
IPC, Main	ICM	Ý	Ý
IPC, Main and Secondary	IC	Ý	Ý
IPC, Secondary	ics	Ϋ́	Ϋ́
Journal Type	JT	Ý	Ý
Language	LA	Ϋ́	Ϋ́
National Patent Classification	NCL	Ý	Ý
Other Source	OS	Ý	Ϋ́
Patent Application Country	AC	Ϋ́	Ϋ́
Patent Application Country, Basic	AC.B	Ý (12)	Ϋ́
Patent Application Date	AD AD	Y (12)	Ϋ́
Patent Application Date, Basic	AD.B	Y (13)	Ϋ́
Patent Application Information	AI.	Y (14,15)	Ϋ́
Patent Application Information, Basic	AI.B	Y (15,16)	Ϋ́
Patent Application Number	AP	Y (15)	Ϋ́
Patent Application Number, Basic	AP.B	Y (15,17)	Ϋ́
Patent Application Number, Basic Patent Application and Priority Number	APPS		N
	APPS.B	Y (15,18)	N N
Patent Application and Priority Number, Basic		Y (15,19) Y	Y
Patent Application Year	AY		
Patent Application Year, Basic	AY.B	Y (20)	Y
Patent Assignee	PA	Y (24)	Y
Patent Countries	PCS	Y (21)	N
Patent Countries, Basic	PCS.B	Y (22)	N
Patent Country	PC PC P	Y (22)	Y
Patent Country, Basic	PC.B	Y (23)	Y
Patent Country Count	CYC	Y (24)	N
Patent Information	PI	Y (15,25)	Y
Patent Information, Basic	PI.B	Y (15,26)	Y
Patent Kind Code	PK	Υ (27)	Y
Patent Kind Code, Basic	PK.B	Y (27)	Y
Patent Number	PN	Y (15)	Y
	PATS	Y (15,28)	N

### SELECT, ANALYZE, and SORT Fields (cont'd)

Field Name	Field Code	ANALYZE/ SELECT	SORT
Patent Number, Basic	PN.B	Y (15,29)	Y
	PATS.B	Y (15,30)	N
Patent Number Count	PNC	Y (31)	N
Patent Number/Kind Code	PNK	Υ	Υ
Patent Number/Kind Code, Basic	PNK.B	Υ	Υ
Priority Application Country	PRC	Υ	Υ
Priority Application Country, Basic	PRC.B	Y (32)	Y
Priority Application Date	PRD	Υ	Y
Priority Application Date, Basic	PRD.B	Y (33)	Υ
Priority Application Information	PRAI	Y (15,34)	Υ
Priority Application Information, Basic	PRAI.B	Y (15,35)	Υ
Priority Application Number	PRN	Y (15)	Υ
Priority Application Number, Basic	PRN.B	Y (15,36)	Υ
Priority Application Year	PRY	Υ `	Υ
Priority Application Year, Basic	PRY.B	Y (37)	Υ
Publication Date	PD	Υ`΄	Υ
Publication Date, Basic	PD.B	Y (38)	Υ
Publication Year	PY	Υ`΄	Υ
Publication Year, Basic	PY.B	Y (39)	Υ
Source of Document	so	Υ'΄	N
Supplementary Term	ST	Υ	N
Title	Ti	Y (default)	Y
Treatment Code	TC	Y (40)	Y

- (1) SELECT HIT AN may be used to restrict terms extracted to those that match the search expression used to create the answer set.
- Appends /BI to the terms created by SELECT.
- (n) may be a single number, range, or a list of numbers separated by a space or comma. (3)
- Selects or analyzes cited reference accession number in CAplus and appends /AN to the terms created by SELECT.
- Selects or analyzes cited reference accession number in MEDLINE and appends /AN to the terms created by SELECT. (5)
- Selects or analyzes cited reference author name and appends /RAU to the terms created by SELECT.
- Selects CODEN and appends /ISN to the terms created by SELECT. (7)
- Appends /DS to the terms created by SELECT. (8)
- Appends /AN to the terms created by SELECT.
- (10) Selects or analyzes the CODEN and appends /ISN to the terms created by SELECT.
- (11) Selects or analyzes IC, ICA, and ICI and appends /IPC to the terms created by SELECT.
- (12) Appends /AC to the terms created by SELECT.
- (13) Appends /AD to the terms created by SELECT.
- (14) Selects or analyzes Patent Application Number and appends /AP to the terms created by SELECT.
- (15) Enter SET PATENT DERWENT at an arrow prompt (=>) to SELECT patent, application, and priority numbers in Derwent format.
- (16) Selects or analyzes Basic Patent Application Number and appends /AP to the terms created by SELECT.
- (17) Appends /AP to the terms created by SELECT.
- (18) Selects or analyzes AP and PRN and appends /APPS to the terms created by SELECT.(19) Selects or analyzes AP.B and PRN>B and appends /APPS to the terms created by SELECT.
- (20) Appends /AY to the terms created by SELECT.
- (21) Selects or analyzes country codes from PI and DS and appends /PCS to the terms created by SELECT.
- (22) Selects or analyzes country codes from PI.B and DS.B and appends /PCS to the terms created by SELECT.
- (23) Appends /PC to the terms created by SELECT.
- (24) Appends /CY.CNT to the terms created by SELECT.
- (25) Selects or analyzes the Patent Number and appends /PN to the terms created by SELECT.
- (26) Selects or analyzes the Basic Patent Number and appends /PN to the terms created by SELECT.
- (27) Appends /PK to the terms created by SELECT.
- (28) Selects or analyzes the Patent Number and appends /PATS to the terms created by SELECT.
- (29) Appends /PN to the terms created by SELECT.
- (30) Selects or analyzes the Basic Patent Number and appends /PATS to the terms created by SELECT.
- (31) Appends /PN.CNT to the terms created by SELECT.
- (32) Appends /PRC to the terms created by SELECT.
- (33) Appends /PRD to the terms created by SELECT.
- (34) Selects Priority Number and appends /PRN to the terms created by SELECT.
- (35) Selects Basic Priority Number and appends /PRN to the terms created by SELECT.
- (36) Appends /PRN to the terms created by SELECT.
- (37) Appends /PRY to the terms created by SELECT.
- (38) Appends /PD to the terms created by SELECT.
- (39) Appends /PY to the terms created by SELECT.
- (40) Appends /DT to the terms created by SELECT.

### Sample Record

**DISPLAY IALL** 

ACCESSION NUMBER: 112:36458 LMARPAT Full-text

TITLE: Preparation of chiral statine analogs via aldol

condensation of acetoxytriarylethanols with amino acid

aldehyde derivatives

INVENTOR(S): Devant, Ralf U.; Radunz, Hans Eckart
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 6 pp. CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

INT. PATENT CLASSIF.:

INITIAL CLASS: C07C0101-30 [ICM,4]; C07C0125-065 [ICS,4]; C07D0263-24

[ICS, 4]

RECLASSIFICATION: C07C0227-32 [I,A]; C07C0229-22 [I,A]; C07C0229-34

[I,A]; C07C0271-22 [I,A]; C07D0263-24 [I,A];

C07D0333-16 [I,A]

CLASSIFICATION: 34-2 (Amino Acids, Peptides, and Proteins)

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

DE 3743225 A1 19890629 DE 1987-3743225 19871219
PRIORITY APPLN. INFO:: DE 1987-3743225 19871219

OTHER SOURCE(S): MARPAT 112:36458

**ABSTRACT:** 

INDEX TERM:

Statine derivs. R4CH2CH(NHR3)CH(OR2)CH2CO2R1 [I; R1 = H, C1-5 alkyl; R2 = H, C1-5 alkyl, COR5; R3 = H, protecting group; R4 = C1-5 alkyl, (substituted) Ph, cyclohexyl; R5 = C1-5 alkyl], useful as renin inhibitor intermediates, were prepared enantioselectively by condensation of AcOCHR6CR7R8OH (R6-R8 = C6-10 aryl) with R4CH2C(NHR3)CHO followed by hydrolysis and transesterification. Thus, (S)-2-acetoxy-1,1,2-triphenylethanol in THF at -78° was treated with (Me2CH)2NLi, and the mixture was stirred 1 h at 0°, and recooled to -78°. N-tert-Butoxycarbonyl-(S)-phenylalaninal in THF was added and the mixture was stirred 2 h to give (2S,3S,4S)-(3-hydroxy-4-tert-butyloxycarbonylamino-5-phenylpentanoyloxy)-1,1,2-triphenylethanol (in a 12:1 ratio over the 3R isomer). The latter was stirred with NaOMe in dioxane/MeOH at 0° to give Me (3S,4S)-3-hydroxy-4-tert-butoxycarbonylamino-5-phenylpentanoate.

SUPPL. TERM: renin inhibitor intermediate statine analog; amino acid

statine analog prepn; aldol condensation enantioselective

amino acid aldehyde

INDEX TERM: Aldol condensation

(of acetoxytriarylethanol derivs. with amino acid

aldehyde derivs.)

INDEX TERM: Asymmetric synthesis and induction

(of statine derivs., via aldol condensation of acetoxytriarylethanols with amino acid aldehydes) 72155-45-4, N-tert-Butoxycarbonyl-(S)-phenylalaninal

124529-58-4, 2-tert-Butoxycarbonylamino-3-(4-

methylcyclohexyl)propanal

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(aldol condensation of, with acetoxytriphenylethanol)

INDEX TERM: 59830-60-3

ROLE: RCT (Reactant); RACT (Reactant or reagent)

(aldol condensation of, with acetoxytriphenylethanol, in

preparation of renin inhibitor intermediate)

INDEX TERM: 95061-51-1, (S)-2-Acetoxy-1,1,2-triphenylethanol ROLE: RCT (Reactant); RACT (Reactant or reagent)

(aldol condensation of, with phenylalaninal)

INDEX TERM: 124529-60-8P 124529-62-0P ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and aldol condensation of, with phenylalaninal derivative, in preparation of intermediate for rennin inhibitor) INDEX TERM: 118219-44-6P 124529-59-5P 124529-63-1P ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and methanolysis of) INDEX TERM: 124529-61-9P ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and methanolysis of, in preparation of rennin inhibitor intermediate) 123689-40-7P INDEX TERM: ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of, as intermediate for renin inhibitor) INDEX TERM: 72155-54-5P 101669-80-1P ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of, as renin inhibitor intermediate) INDEX TERM: 118219-42-4P ROLE: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as renin inhibitor intermediate) INDEX TERM: 49642-07-1DP, Statine, derivs. ROLE: SPN (Synthetic preparation); PREP (Preparation) (preparation of, via aldol condensation of amino acid aldehydes with acetoxytriarylethanols) INDEX TERM: 2786-07-4, 2-Thienyllithium ROLE: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with mandelic acid and acetyl chloride) INDEX TERM: 4294-57-9, p-Tolylmagnesium bromide ROLE: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with methylmandelic acid and acetyl chloride) INDEX TERM: 75-36-5, Acetyl chloride ROLE: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with methylmandelic acid and tolylmagnesium bromide, in preparation of renin inhibitor intermediate) INDEX TERM: 17199-29-0, S-Mandelic acid ROLE: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with thienyllithium and acetyl chloride) INDEX TERM: 75172-62-2 ROLE: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with tolylmagnesium bromide and acetyl chloride, in preparation of renin inhibitor intermediate) REFERENCE COUNT: THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. REFERENCE(S): (1) Anon; DE 3628650 A1 CAPLUS MSTR 1 = OH / alkoxy <containing 1-5 C> G1= OH / alkoxy <containing 1-5 C> / alkylcarbonyloxy <containing 1-5 C> G3 = NH2 / 11

**н**¥——G6

```
G4
       = alkyl <containing 1-5 C> /
         Ph (opt. substd. by 1 or more G5) /
         cyclohexyl (opt. substd. by 1 or more G5)
G5
       = alkyl <containing 1-4 C> /
         alkoxy <containing 1-4 C> / halo / OH
G6
       = R <"protecting group"> / (Examples: CO2CH2Ph /
         CO2Bu-t / CH2Ph / 28)
      H2C-
                <del>_2</del>6 (0)
Patent location:
                             claim 1
MSTR 2
G1
       = aryl <containing 6-10 C> (opt. substd.) /
         heteroaryl <containing 6-10 C> (opt. substd.) /
         (Examples: 11 / thienyl / pyridyl / naphthyl)
 162 - G3
G2
       = phenylene
G3
       = halo / Cl / F / OH / Me / OMe / NO2
G4
       = aryl <containing 6-10 C> (opt. substd.) /
         heteroaryl <containing 6-10 C> (opt. substd.) /
         (Examples: 13 / thienyl / pyridyl / naphthyl)
 1<sup>6</sup>6—G3
G5
       = aryl <containing 6-10 C> (opt. substd.) /
         heteroaryl <containing 6-10 C> (opt. substd.) /
         (Examples: 15 / thienyl / pyridyl / naphthyl)
 157-G3
G6
       = phenylene
G7
       = phenylene
Patent location:
                             claim 1
  MSTR 3
G3
       = NH2 / 11
 ₽₽—G6
G4
       = alkyl <containing 1-5 C> /
         Ph (opt. substd. by 1 or more G5) /
         cyclohexyl (opt. substd. by 1 or more G5)
G5
       = alkyl <containing 1-4 C> /
         alkoxy <containing 1-4 C> / halo / OH
       = R <"protecting group"> / (Examples: CO2CH2Ph /
G6
         CO2Bu-t / CH2Ph / 28)
```

```
H<sub>2</sub>C — 0 — 2 G (0)
```

Patent location:

claim 1

#### MSTR 4

G2 = OH / alkoxy <containing 1-5 C> / alkylcarbonyloxy <containing 1-5 C>

G3 = NH2 / 11

### **H**¥—G6

- G4 = alkyl <containing 1-5 C> /
   Ph (opt. substd. by 1 or more G5) /
   cyclohexyl (opt. substd. by 1 or more G5)
- G5 = alkyl <containing 1-4 C> / alkoxy <containing 1-4 C> / halo / OH
- G6 = R <"protecting group"> / (Examples: CO2CH2Ph / CO2Bu-t / CH2Ph / 28)

G7 = aryl <containing 6-10 C> (opt. substd.) /
heteroaryl <containing 6-10 C> (opt. substd.) /
(Examples: 35 / thienyl / pyridyl / naphthyl)

#### 3G10-G13

G8 = aryl <containing 6-10 C> (opt. substd.) /
 heteroaryl <containing 6-10 C> (opt. substd.) /
 (Examples: 37 / thienyl / pyridyl / naphthyl)

### 3<sup>911-G13</sup>

G9 = aryl <containing 6-10 C> (opt. substd.) /
 heteroaryl <containing 6-10 C> (opt. substd.) /
 (Examples: 39 / thienyl / pyridyl / naphthyl)

#### 3G12-G13

G10 = phenylene G11 = phenylene G12 = phenylene

G13 = halo / Cl / F / OH / Me / OMe / NO2

Patent location: claim 1

#### **DISPLAY QHIT (SET MPTASSEMBLY ON = SYSTEM DEFAULT)**

MSTR 1 Assembled

$$60 \underbrace{\begin{array}{c} 62 \\ 59 \\ 57 \end{array}}_{56} \text{CH}_2 - \underbrace{\begin{array}{c} \text{G3} \\ \text{CH} \\ \text{CH} \\ \text{CH} \\ \text{CH} \\ \text{CH} \\ \text{CH} \\ \text{CH}_2 \\ \text{C} \\ \text{G1} \\ \text{CH}_3 \\ \text{C} \\ \text{C} \\ \text{G1} \\ \text{C} \\$$

56, 57, 59, 60, 62: opt. substd. by 1 or more G5 Patent location: claim 1

MSTR 3 Assembled

$$47 \underbrace{49}_{44} CH_2 - CH - CH = 0$$

43, 44, 46, 47, 49: opt. substd. by 1 or more G5 Patent location: claim 1

MSTR 4 Assembled

$$70 \underbrace{ \begin{array}{c} \text{G3} & \text{G2} & \text{O} & \text{G7} & \text{G9} \\ \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{CH}_2 - \text{C}_2 - \text{O}_2 - \text{CH}_2 - \text{C}_2 - \text{OH}_2 \\ \text{G8} \end{array} }_{\text{G8}}$$

66, 67, 69, 70, 72: opt. substd. by 1 or more G5 Patent location: claim 1

#### **DISPLAY QHITEXG**

MSTR 1 Assembled

56, 57, 59, 60, 62: opt. substd. by 1 or more G5

Additional displayed G-groups:

G1 = OH / alkoxy <containing 1-5 C>

G2 = OH / alkoxy <containing 1-5 C> / alkylcarbonyloxy <containing 1-5 C>

G3 = NH2 / 11

**н**ұ—\_\_\_\_ G6

Patent location: claim 1

#### MSTR 3 Assembled

$$47 \underbrace{49}_{44}^{\text{CH}_2-\text{CH-CH}}^{\text{G3}}_{\text{CH-CH}}^{\text{CH}} \circ$$

43, 44, 46, 47, 49: opt. substd. by 1 or more G5

Additional displayed G-groups: = NH2 / 11G3

**₽₽**—G6

Patent location: claim 1

### MSTR 4 Assembled

$$70 \overbrace{ \begin{array}{c} 72 \\ 69 \\ 67 \end{array} }^{\text{G3}} \underbrace{ \begin{array}{c} \text{G2} \\ \text{CH}_{2} \\ \text{CH}_{-} \\$$

66, 67, 69, 70, 72: opt. substd. by 1 or more G5

Additional displayed G-groups:

= OH / alkoxy <containing 1-5 C> /alkylcarbonyloxy <containing 1-5 C>

G3 = NH2 / 11

**₽₽**—G6

G7 = aryl <containing 6-10 C> (opt. substd.) / heteroaryl <containing 6-10 C> (opt. substd.) / (Examples: 35 / thienyl / pyridyl / naphthyl)

3g10-G13

G8 = aryl <containing 6-10 C> (opt. substd.) / heteroaryl <containing 6-10 C> (opt. substd.) / (Examples: 37 / thienyl / pyridyl / naphthyl)

3<sup>6</sup>11–613

G9 = aryl <containing 6-10 C> (opt. substd.) / heteroaryl <containing 6-10 C> (opt. substd.) / (Examples: 39 / thienyl / pyridyl / naphthyl)

3**G**12—G13

Patent location: claim 1

In North America

CAS Customer Center: P.O. Box 3012 Columbus, Ohio 43210-0012

U.S.A.

800-753-4227 (North America) Phone: 614-447-3731 (worldwide)

F-mail· help@cas.org Internet: www.cas.org

In Europe

CAS Customer Center EMEA

represented by FIZ Karlsruhe - Leibniz-Institute for Information Infrastructure Hermann-von-Helmholtz-Platz 1

76344 Eggenstein-Leopoldshafen

Germany

Phone: +49-721-9588 3155 EMEAhelp@cas.org Internet: www.fiz-karlsruhe.de

Japan

In Japan

Information)

Nakai Building

Tokyo 113-0021

JAICI

+81-3-5978-3601 (Technical Service) Phone: +81-3-5978-3621 (Customer Service) F-mail: support@jaici.or.jp (Technical Service) customer@jaici.or.jp (Customer

(Japan Association for International Chemical

6-25-4 Honkomagome, Bunkyo-ku

Service)

Internet: www.jajci.or.jp