

<b>Subject Coverage</b>	<ul style="list-style-type: none"> <li>• Markush patents covered in CAplus<sup>SM</sup></li> <li>• Organo or organometallic molecules</li> <li>• Polymers not included</li> </ul>																				
<b>File Type</b>	Markush Structure, Training																				
<b>Features</b>	<table border="0"> <tr> <td>Thesaurus</td> <td>None</td> <td></td> <td></td> </tr> <tr> <td>Alerts (SDIs)</td> <td>None</td> <td></td> <td></td> </tr> <tr> <td><a href="#">CAS Registry Number<sup>®</sup> Identifiers</a></td> <td><input checked="" type="checkbox"/></td> <td>Page Images</td> <td><input type="checkbox"/></td> </tr> <tr> <td><a href="#">Keep &amp; Share</a></td> <td><input checked="" type="checkbox"/></td> <td>SLART</td> <td><input type="checkbox"/></td> </tr> <tr> <td>Learning Database</td> <td><input checked="" type="checkbox"/></td> <td>Structures</td> <td><input checked="" type="checkbox"/></td> </tr> </table>	Thesaurus	None			Alerts (SDIs)	None			<a href="#">CAS Registry Number<sup>®</sup> Identifiers</a>	<input checked="" type="checkbox"/>	Page Images	<input type="checkbox"/>	<a href="#">Keep &amp; Share</a>	<input checked="" type="checkbox"/>	SLART	<input type="checkbox"/>	Learning Database	<input checked="" type="checkbox"/>	Structures	<input checked="" type="checkbox"/>
Thesaurus	None																				
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<a href="#">Keep &amp; Share</a>	<input checked="" type="checkbox"/>	SLART	<input type="checkbox"/>																		
Learning Database	<input checked="" type="checkbox"/>	Structures	<input checked="" type="checkbox"/>																		
<b>Record Content</b>	<ul style="list-style-type: none"> <li>• Markush structures found in the claims and often the disclosure of the patent, bibliographic information, patent family information, cited references</li> <li>• In-depth substance and subject indexing including CAS Registry Numbers<sup>®</sup>, and an abstract, all of which are displayable</li> <li>• The structures are searchable</li> <li>• Document information can be searched in CA<sup>SM</sup> and CAplus</li> </ul>																				
<b>File Size</b>	569 records (02/16)																				
<b>Coverage</b>	Selected Markush structure records for patents found in CAplus with the patent publication year of 1988-1989																				
<b>Updates</b>	None																				
<b>Language</b>	English																				
<b>Database Producer</b>	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) Fax: 614-447-3751 Email: <a href="mailto:help@cas.org">help@cas.org</a> Copyright Holder																				

**Sources**

Selected Markush patents found in CAplus

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**User Aids**

- Online Helps (HELP DIRECTORY lists all help messages available)
  - STNGUIDE
- 

**Cluster**

- LEARNING

STN Database Cluster Information:

<http://www.stn-international.com/en/customersupport/customer-support#cluster+%7C+subjects+%7C+features>

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**Related Databases**

MARPAT

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## 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

(1) Only structure-related text terms are included; terms from the CPlus Basic Index are not searchable.

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

## 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

(1) 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.

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

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

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

**DISPLAY Formats (cont'd)**

<b>Format</b>	<b>Content</b>	<b>Examples</b>
PA (CS) PI (1) PI.B (PN.B) (1,2) PN PNC (PN.CNT) (2) PNK PNK.B PRAI (PRN) (1) PRAI.B (PRN.B)(1) PY (2) PY.B (2) RE (3) RETABLE (2,3) RE.CNT (REC) (3) RL (4) RN (2) SO ST SX (2,5) TI	Patent Assignee Patent Information Table Patent Information, Basic Patent Number Patent Number Count Patent Number/Kind Code Patent Number/Kind Code, Basic Priority Application Information Priority Application Information, Basic Publication Year Publication Year, Basic Cited References Cited References Table Citing Document's Reference Count Index Term and CAS role CAS Registry Numbers Source Supplementary Term (CA keyword) CA Section Cross-Reference Code Title of Document	D PA D TI PI D PI.B D PN D PNC D PNK D PNK.B D AI PRAI D PRAI.B D PY D TI PY.B D TI RE D TI AU RETABLE D REC D RL D AN RN D TI AU SO D ST D TI SX D TI MSTR
ABS ALL (1,4)  APPS (1) APPS.B (1) BIB (1)  CAN CBIB DALL (1,4) DMAX (1,4) FAM (1)  FAN FBIB (1) IABS IALL (1,4) IBIB (1) IC IDE IMAX (1,4) IND (4) IPC ISTD (1) MAX (1,4) OBIB (1) OIBIB (1) PATS (1) SAM (4) SBIB (1)  SCAN (3,4,6)  SIBIB (1) STD (1)	GI, AB AN, TI, IN, PA, SO, DT, LA, NCL, CC, FAN.CNT, PI, PRAI, OS, GI, AB, ST, IT, RL, RE.CNT, RE, MSTR AI, PRAI AI.B, PRAI.B AN, TI, IN, PA, SO, DT, LA, FAN.CNT, PI, PRAI, OS, RE.CNT (BIB is the default) List of CA Abstract Numbers (no L-number header) AN, plus Compressed Bibliographic Data ALL, delimited for post-processing MAX, delimited for post-processing AN, FAN.CNT, PI for the accession number, plus PI for other family accession numbers Family Accession Number (AN, FAN.CNT, FAN) BIB plus PI for other family accession numbers ABS, with text labels ALL, indented with text labels BIB, indented with text labels International Patent Classification, Main and Secondary AN, MSTR MAX, indented with text labels IPC, NCL, CC, ST, IT, RL International Patent Classifications (IC (ICM, ICS), ICA, ICI) STD, indented with text labels ALL, plus PI for other family accession numbers BIB, Original (AN, TI, IN, PA, SO, PI, DS, AI, PRAI, DT, LA, OS) OBIB, indented with text labels SO, PI IPC, NCL, CC, SX, TI, ST, IT, and FQHIT BIB, without RE.CNT (AN, DN, TI, AU, IN, CS, PA, SO, PB, DT, LA, FAN.CNT, PI, PRAI, OS) IPC, NCL, CC, TI, ST, IT, RL, FQHIT (random display, no answer numbers) SBIB, indented with text labels AN, TI, IN, PA, SO, DT, LA, FAN.CNT, PI, PRAI, NCL, OS, RE.CNT	D ABS D L2 1-7 ALL  D APPS D APPS.B D 1-3 BIB HIT  D CAN DISPLAY L1 1 CBIB D DALL D MAX D FAM  D FAN D FBIB D IABS D IALL D IBIB D IC D IDE D IMAX D TI IND D IPC D ISTD D MAX D OBIB D OIBIB D PATS DIS SAM 1-5 D 1 3 SBIB  D SCAN  D SIBIB 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	Y	Y
CA Classification Code (section and subsection)	CC	Y	Y
CA Section Cross-Reference Code	SX	Y	Y
CAS Registry Number	RN	Y (2)	N
CAS Role	RL	Y	N
Cited References	RE	Y	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	Y
	REC	Y	Y
Cited Reference Patent Number	RPN	Y	N
Cited Reference Publication Year	RPY	Y	N
Cited Reference Work Title	RWK	Y	N
CODEN	CODEN	Y (7)	Y
Controlled Term	CT	Y	N
Corporate Source (Patent Assignee)	CS	Y	Y
Country Name of Author	CYA	Y	Y
Designated State	DS	Y	N
Designated States, Basic	DS.B	Y (8)	N
Document Type	DT	Y	Y
Family Accession Number	FAN	Y (9)	N
File Segment	FS	Y	Y
Index Term	IT	Y	N
International Standard (Document) Number	ISN	Y (10)	N
International Standard Serial Number	ISSN	Y	Y
Inventor Name	IN	Y	Y
IPC	IPC	Y (11)	Y
IPC, Additional or Supplementary	ICA	Y	Y
IPC, Index or Complementary	ICI	Y	Y
IPC, Main	ICM	Y	Y
IPC, Main and Secondary	IC	Y	Y
IPC, Secondary	ICS	Y	Y
Journal Type	JT	Y	Y
Language	LA	Y	Y
National Patent Classification	NCL	Y	Y
Other Source	OS	Y	Y
Patent Application Country	AC	Y	Y
Patent Application Country, Basic	AC.B	Y (12)	Y
Patent Application Date	AD	Y	Y
Patent Application Date, Basic	AD.B	Y (13)	Y
Patent Application Information	AI	Y (14,15)	Y
Patent Application Information, Basic	AI.B	Y (15,16)	Y
Patent Application Number	AP	Y (15)	Y
Patent Application Number, Basic	AP.B	Y (15,17)	Y
Patent Application and Priority Number	APPS	Y (15,18)	N
Patent Application and Priority Number, Basic	APPS.B	Y (15,19)	N
Patent Application Year	AY	Y	Y
Patent Application Year, Basic	AY.B	Y (20)	Y
Patent Assignee	PA	Y	Y
Patent Countries	PCS	Y (21)	N
Patent Countries, Basic	PCS.B	Y (22)	N
Patent Country	PC	Y	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	Y	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	Y	Y
Patent Number/Kind Code, Basic	PNK.B	Y	Y
Priority Application Country	PRC	Y	Y
Priority Application Country, Basic	PRC.B	Y (32)	Y
Priority Application Date	PRD	Y	Y
Priority Application Date, Basic	PRD.B	Y (33)	Y
Priority Application Information	PRAI	Y (15,34)	Y
Priority Application Information, Basic	PRAI.B	Y (15,35)	Y
Priority Application Number	PRN	Y (15)	Y
Priority Application Number, Basic	PRN.B	Y (15,36)	Y
Priority Application Year	PRY	Y	Y
Priority Application Year, Basic	PRY.B	Y (37)	Y
Publication Date	PD	Y	Y
Publication Date, Basic	PD.B	Y (38)	Y
Publication Year	PY	Y	Y
Publication Year, Basic	PY.B	Y (39)	Y
Source of Document	SO	Y	N
Supplementary Term	ST	Y	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.
- (2) Appends /BI to the terms created by SELECT.
- (3) (n) may be a single number, range, or a list of numbers separated by a space or comma.
- (4) Selects or analyzes cited reference accession number in CAPlus and appends /AN to the terms created by SELECT.
- (5) Selects or analyzes cited reference accession number in MEDLINE and appends /AN to the terms created by SELECT.
- (6) Selects or analyzes cited reference author name and appends /RAU to the terms created by SELECT.
- (7) Selects CODEN and appends /ISN to the terms created by SELECT.
- (8) Appends /DS to the terms created by SELECT.
- (9) 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
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DE 3743225	A1	19890629	DE 1987-3743225	19871219
PRIORITY APPLN. INFO.:			DE 1987-3743225	19871219

OTHER SOURCE(S): MARPAT 112:36458

### ABSTRACT:

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-butylloxycarbonylamino-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)  
INDEX TERM: 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

## LMARPAT

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)

INDEX TERM: 123689-40-7P  
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)

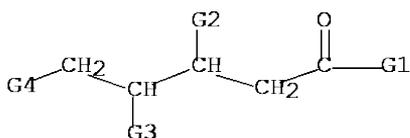
INDEX TERM: 17199-29-0, S-Mandelic acid  
ROLE: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with thienyllithium and acetyl chloride)

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: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS  
RECORD.

REFERENCE(S): (1) Anon; DE 3628650 A1 CAPLUS

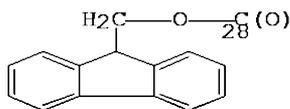
## MSTR 1



G1 = OH / alkoxy <containing 1-5 C>  
G2 = OH / alkoxy <containing 1-5 C> /  
alkylcarbonyloxy <containing 1-5 C>  
G3 = NH<sub>2</sub> / 11

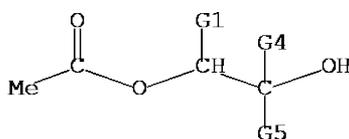


- G4 = alkyl <containing 1-5 C> /  
Ph (opt. substd. by 1 or more G5) /  
cyclohexyl (opt. substd. by 1 or more G5)
- G5 = alkyl <containing 1-4 C> /  
alkoxy <containing 1-4 C> / halo / OH
- G6 = R <"protecting group"> / (Examples: CO<sub>2</sub>CH<sub>2</sub>Ph /  
CO<sub>2</sub>Bu-t / CH<sub>2</sub>Ph / 28)

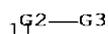


Patent location: claim 1

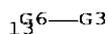
MSTR 2



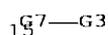
- G1 = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 11 / thienyl / pyridyl / naphthyl)



- G2 = phenylene
- G3 = halo / Cl / F / OH / Me / OMe / NO<sub>2</sub>
- G4 = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 13 / thienyl / pyridyl / naphthyl)



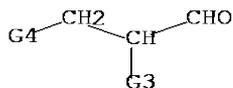
- G5 = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 15 / thienyl / pyridyl / naphthyl)



- G6 = phenylene
- G7 = phenylene

Patent location: claim 1

MSTR 3

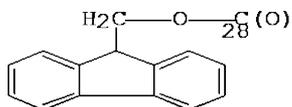


- G3 = NH<sub>2</sub> / 11



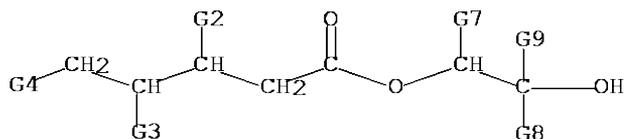
- G4 = alkyl <containing 1-5 C> /  
Ph (opt. substd. by 1 or more G5) /  
cyclohexyl (opt. substd. by 1 or more G5)
- G5 = alkyl <containing 1-4 C> /  
alkoxy <containing 1-4 C> / halo / OH
- G6 = R <"protecting group"> / (Examples: CO<sub>2</sub>CH<sub>2</sub>Ph /  
CO<sub>2</sub>Bu-t / CH<sub>2</sub>Ph / 28)

## LMARPAT



Patent location: claim 1

## MSTR 4



$G_2$  = OH / alkoxy <containing 1-5 C> /

alkylcarbonyloxy <containing 1-5 C>

$G_3$  =  $NH_2$  / 11



$G_4$  = alkyl <containing 1-5 C> /

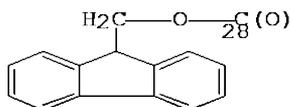
Ph (opt. substd. by 1 or more  $G_5$ ) /

cyclohexyl (opt. substd. by 1 or more  $G_5$ )

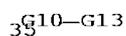
$G_5$  = alkyl <containing 1-4 C> /

alkoxy <containing 1-4 C> / halo / OH

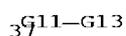
$G_6$  = R <"protecting group"> / (Examples:  $CO_2CH_2Ph$  /  $CO_2Bu-t$  /  $CH_2Ph$  / 28)



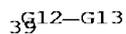
$G_7$  = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 35 / thienyl / pyridyl / naphthyl)



$G_8$  = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 37 / thienyl / pyridyl / naphthyl)



$G_9$  = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 39 / thienyl / pyridyl / naphthyl)



$G_{10}$  = phenylene

$G_{11}$  = phenylene

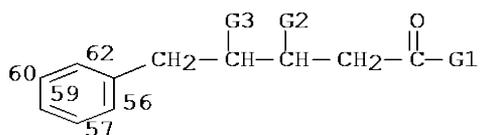
$G_{12}$  = phenylene

$G_{13}$  = halo / Cl / F / OH / Me / OMe /  $NO_2$

Patent location: claim 1

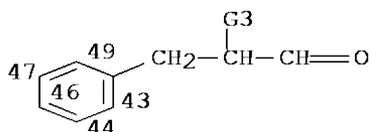
**DISPLAY QHIT (SET MPTASSEMBLY ON = SYSTEM DEFAULT)**

MSTR 1 Assembled



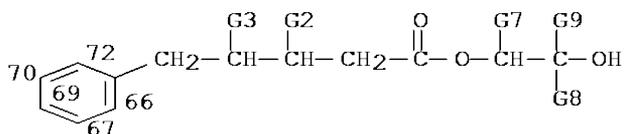
56, 57, 59, 60, 62: opt. substd. by 1 or more G5  
 Patent location: claim 1

MSTR 3 Assembled



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

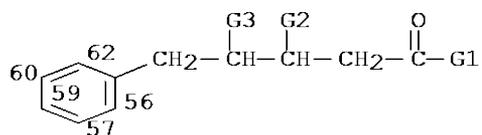
MSTR 4 Assembled



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 &lt;containing 1-5 C&gt;

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

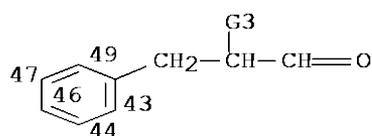
G3 = NH2 / 11



Patent location: claim 1

**LMARPAT**

MSTR 3 Assembled



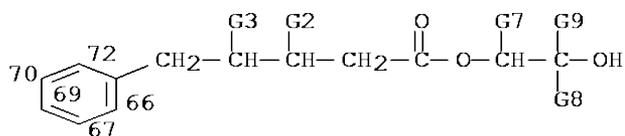
43, 44, 46, 47, 49: opt. substd. by 1 or more G5

Additional displayed G-groups:

G3 = NH<sub>2</sub> / 11

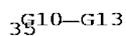
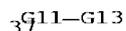
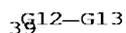
Patent location: claim 1

MSTR 4 Assembled



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

Additional displayed G-groups:

G2 = OH / alkoxy <containing 1-5 C> /  
alkylcarbonyloxy <containing 1-5 C>G3 = NH<sub>2</sub> / 11G7 = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 35 / thienyl / pyridyl / naphthyl)G8 = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 37 / thienyl / pyridyl / naphthyl)G9 = aryl <containing 6-10 C> (opt. substd.) /  
heteroaryl <containing 6-10 C> (opt. substd.) /  
(Examples: 39 / thienyl / pyridyl / naphthyl)

Patent location: claim 1

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