

<b>Subject Coverage</b>	<ul style="list-style-type: none"> <li>Markush structure records for patents found in CAplus<sup>SM</sup></li> <li>Markush structures derived from Institute National de la Propriete Industrielle (INPI) data from 1961 to 1987</li> </ul>															
<b>File Type</b>	Markush structures															
<b>Features</b>	<table border="0"> <tr> <td><a href="#">Alerts (SDIs)</a></td> <td>Every two weeks</td> <td></td> <td></td> <td></td> </tr> <tr> <td><a href="#">CAS Registry Number® Identifiers</a></td> <td><input checked="" type="checkbox"/></td> <td><a href="#">Keep &amp; Share</a></td> <td><input checked="" type="checkbox"/></td> <td>STN® AnaVist™ <input type="checkbox"/></td> </tr> <tr> <td><a href="#">Learning Database</a></td> <td><input checked="" type="checkbox"/></td> <td>Structures</td> <td><input checked="" type="checkbox"/></td> <td>STN Easy® <input type="checkbox"/></td> </tr> </table>	<a href="#">Alerts (SDIs)</a>	Every two weeks				<a href="#">CAS Registry Number® Identifiers</a>	<input checked="" type="checkbox"/>	<a href="#">Keep &amp; Share</a>	<input checked="" type="checkbox"/>	STN® AnaVist™ <input type="checkbox"/>	<a href="#">Learning Database</a>	<input checked="" type="checkbox"/>	Structures	<input checked="" type="checkbox"/>	STN Easy® <input type="checkbox"/>
<a href="#">Alerts (SDIs)</a>	Every two weeks															
<a href="#">CAS Registry Number® Identifiers</a>	<input checked="" type="checkbox"/>	<a href="#">Keep &amp; Share</a>	<input checked="" type="checkbox"/>	STN® AnaVist™ <input type="checkbox"/>												
<a href="#">Learning Database</a>	<input checked="" type="checkbox"/>	Structures	<input checked="" type="checkbox"/>	STN Easy® <input type="checkbox"/>												
<b>Record Content</b>	Markush structures of organic or organometallic molecules are searchable. Patent reference information is displayable.															
<b>File Size</b>	More than 554,536 patent records (9/2021)															
<b>Coverage</b>	1961 to the present															
<b>Updates</b>	Daily															
<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															
<b>Sources</b>	<ul style="list-style-type: none"> <li>Patents found in CAplus with the patent publication year of 1988 to the present</li> <li>English language patents from 1984-1987 (selective coverage)</li> <li>French and German patents from 1986-1987 (selective coverage)</li> <li>Japanese patents from 1987 (selective coverage)</li> <li>Russian patents published after January 10, 2000</li> <li>Korean patents from 2008 to the present</li> <li>INPI data from 1961 to 1987</li> </ul>															
<b>User Aids</b>	<ul style="list-style-type: none"> <li>Support and training materials are available on the web: <a href="http://www.cas.org">www.cas.org</a></li> <li>Online Helps (HELP DIRECTORY lists all help messages available)</li> <li>STNGUIDE</li> </ul>															
<b>Clusters</b>	<ul style="list-style-type: none"> <li>CASLINK</li> <li>HCASLINK</li> <li>STRUCTURE</li> <li><a href="#">STN Database Clusters</a> information (PDF).</li> </ul>															
<b>Related Databases</b>	LMARPAT <sup>SM</sup>															
<b>Pricing</b>	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 CAplus Accession Number Entry Date (2) Update Date (2)	/AN /ANPL /ED /UP	S 118:93622/AN S 2000:271958/ANPL S 19990305/ED S L1 AND UP>=19990100	AN ANPL Not displayed Not displayed

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

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

## Limiting Search Codes

Only an L-number for an answer set created in MARPAT may be limited.

Search Field Name	Search Code	Search Examples	Display Codes
Answers completely iterated Answers incompletely iterated	/COMPLETE /INCOMPLETE	S L4/COM (1) S L4/INC (1)	Not displayed Not displayed

(1) The code may be abbreviated to the first three letters.

## 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 Search a fixed sample of an answer set created by a search in MARPAT	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 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 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) (1)	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 (SC)	CA Classification Code (CA section and section cross-references)	D CC
CO	CODEN	D CO, D ISN
CT (2)	Controlled Term	D CT
CYA (2)	Country of Author	D CYA
CYC (CY.CNT) (2)	Patent Country Count	D CYC
DN	Document Number	D DN
DS (2)	Designated States	D PI DS
DS.B (2)	Designated States, Basic	D DS.B
DT (TC)	Document Type	D DT
FAN	Family Accession Number	D FAN
FS (2)	File Segment (Section Group)	D FS
GI (3)	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	D IN
ISN (ISSN) (2)	International Standard (Document) Number	D ISN
IT (4)	Index Term and CAS role	D AN IT
JT (JTA, JTF)	Journal Title	D JT, D JTA, D JTF
LA	Language	D LA
MSTR	All Markush structures and related text	D AN MSTR
MSTR(n) (2)	Markush structure n and its related text	D AN MSTR (1)
NCL	National Patent Classification	D NCL

**DISPLAY Formats (cont'd)**

<b>Format</b>	<b>Content</b>	<b>Examples</b>
PSPI (STI) PSPI.B OS 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 UPP	Patent Status Patent Information Patent Status Patent Information, Basic Other Source 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 Update Date Patent	D PSPI D PSPI.B D OS 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 D UPP
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) PATS.B (1) SAM (4) SBIB (1)  SCAN (3,4,6)  SIBIB (1)	GI, AB AN, TI, IN, PA, SO, DT, LA, NCL, CC, FAN.CNT, PI, PRAI, PSPI, 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, PSPI, 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, PSPI, DT, LA, OS) OBIB, indented with text labels SO, PI SO, PI for basic patents 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, PSPI, OS) IPC, NCL, CC, TI, ST, IT, RL, FQHIT (random display, no answer numbers) SBIB, indented with text labels	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 D PATS.B DIS SAM 1-5 D 1 3 SBIB  D SCAN  D SIBIB

**DISPLAY Formats (cont'd)**

Format	Content	Examples
STD(1)	AN, TI, IN, PA, SO, DT, LA, FAN.CNT, PI, PRAI, PSPI, NCL, OS, RE.CNT	D STD
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
```

**MARPAT****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).

<b>Field Name</b>	<b>Field Code</b>	<b>ANALYZE/ SELECT</b>	<b>SORT</b>
Abstract Text	AB	Y	N
Accession Number	AN	Y <b>(1)</b>	N
Author (Inventor)	AU (IN)	Y	Y
CA Classification Code (section and subsection)	CC (SC)	Y	Y
CA Section Cross-Reference Code	SX	Y	Y
CAS Registry Number	RN	Y <b>(2)</b>	N
CAS Role	RL	Y	N
Cited References	RE	Y	N
Cited Reference(n)	RE(n)	Y <b>(3)</b>	N
Cited Reference Accession Number in CPlus	RAN.CAPLUS	Y <b>(4)</b>	N

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

Field Name	Field Code	ANALYZE/ SELECT	SORT
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 (RIN)	Y (6)	N
Cited Reference Count	RE.CNT (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 (TC)	Y (10)	Y
Family Accession Number	FAN	Y (9)	N
File Segment	FS	Y	Y
Index Term	IT	Y	N
International Standard Serial Number	ISSN (ISN)	Y (7)	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 Title	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 (CY.CNT)	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
Patent Number, Basic	PN.B	Y (15,29)	Y
	PATS.B	Y (15,30)	N

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

Field Name	Field Code	ANALYZE/ SELECT	SORT
Patent Number Count	PNC (PN.CNT)	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

- (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) 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) Appends /DT 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.



## Sample Record

## DISPLAY IALL (GTEXT=ON)

ACCESSION NUMBER: \*\*\*132:264964\*\*\* MARPAT  
 TITLE: Preparation of aromatic hydroxythiols from bis-diazonium salts  
 INVENTOR(S): Zhang, Mingbao; Ryckman, David; Mac, Eric  
 PATENT ASSIGNEE(S): AlliedSignal Inc., USA  
 SOURCE: U.S., 5 pp.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 INITIAL US PAT. CLASS.: 568062000  
 INT. PATENT CLASSIF.:  
 INITIAL CLASS: C07C0319-02 [ICM,7]  
 RECLASSIFICATION: C07C0319-06 [I]; C07C0319-22 [I]; C07C0319-24 [I];  
 C07C0323-20 [N]; C07C0323-29 [N]  
 US PATENT CLASSIF.: 568/062.000; 548/544.000; 549/062.000; 549/476.000;  
 549/505.000; 568/061.000  
 CLASSIFICATION: 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 Section cross-reference(s): 45  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6054622	A	20000425	US 1998-213144	19981218
WO 2000037439	A1	20000629	WO 1999-US29579	19991215
EP 1140816	A1	20011010	EP 1999-966198	19991215
US 6303822	B1	20011016	US 2000-515355	20000229
PRIORITY APPLN. INFO.:			US 1998-213144	19981218
			WO 1999-US29579	19991215

## PATENT STATUS PATENT INFORMATION:

PATENT NO.	KIND	STATUS	STATUS DATE
US 6054622	A	Dead	20201106
WO 2000037439	A1	Dead	20201106
EP 1140816	A1	Dead	20201106
US 6303822	B1	Dead	20201107

OTHER SOURCE(S): CASREACT 132:264964

GRAPHIC IMAGE: Diagram(s) available in offline prints or printed CA through Vol 151.

## ABSTRACT:

Arom. hydroxythiols (e.g., 3-hydroxythiophenol) are prepd. in high yield and selectivity by oxidizing an arom. aminothiols (e.g., 3-aminothiophenol) to an aminodisulfide compd., forming a bis-diazonium salt of the aminodisulfide compd., and reacting the bis-diazonium salt with water to form an arom. hydroxyldisulfide compd., which is then reduced to the hydroxythiol.

SUPPL. TERM: hydroxythiophenol prepn; arom hydroxythiol prepn;  
 aminothiophenol oxidn diazotization hydroxylation redn prepn  
 hydroxythiophenol

INDEX TERM: Thiols (organic), reactions  
 Thiols (organic), reactions  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (amino, arom.; prepn. of arom. hydroxythiols from  
 bis-diazonium salts)

INDEX TERM: Thiols (organic), preparation  
 Thiols (organic), preparation  
 ROLE: IMF (Industrial manufacture); SPN (Synthetic  
 preparation); PREP (Preparation)  
 (aryl, arom. hydroxythiols; prepn. of arom. hydroxythiols  
 from bis-diazonium salts)

## MARPAT

## DISPLAY IALL (GTEXT=ON) (cont'd)

INDEX TERM: Diazonium compounds  
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (bis-diazonium salts of aminodisulfide compds.)

INDEX TERM: Thermal decomposition  
 (in the manuf. of arom. hydroxythiols from bis-diazonium salts)

INDEX TERM: Oxidation  
 (liq.-phase; of arom. aminothiols into diamino diaryl disulfides)

INDEX TERM: Hydroxylation  
 (of bis-diazonium salts of arom. aminodisulfide compds.)

INDEX TERM: Diazotization  
 (of diamino arom. disulfides in the manuf. of arom. hydroxythiols)

INDEX TERM: Amines, reactions  
 Amines, reactions  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (thiol, arom.; prepn. of arom. hydroxythiols from bis-diazonium salts)

INDEX TERM: Phenols, preparation  
 Phenols, preparation  
 ROLE: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (thiophenols, arom. hydroxythiols; prepn. of arom. hydroxythiols from bis-diazonium salts)

INDEX TERM: 1121-24-0 45993-54-2 80018-01-5 106949-90-0  
 1025798-13-3 1027055-83-9 1097992-04-5  
 ROLE: PRPH (Prophetic)  
 (Preparation of aromatic hydroxythiols from bis-diazonium salts)

INDEX TERM: 7732-18-5, Water, reactions  
 ROLE: NUU (Other use, unclassified); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)  
 (prepn. of arom. hydroxythiols from bis-diazonium salts)

INDEX TERM: 137-07-5, 2-Aminothiophenol 1193-02-8, 4-Aminothiophenol  
 7632-00-0, Sodium nitrite 22948-02-3, 3-Aminothiophenol  
 ROLE: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of arom. hydroxythiols from bis-diazonium salts)

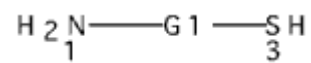
INDEX TERM: 40248-84-8P, 3-Hydroxythiophenol  
 ROLE: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of arom. hydroxythiols from bis-diazonium salts)

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD.

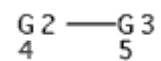
REFERENCE(S): (1) Allen; Org Synth Coll 1943, V1, P580  
 (2) Anon; Gazz Chim Ital 99 by Cabiddu 1969, P1095  
 (3) Anon; J Amer Chem Soc By Djerassi 1955, V77, P568  
 (4) Anon; J Chem Soc by Watson and Dutt 1922, V121, P2414  
 (5) Christidis; US 4948827 1990 CAPLUS  
 (6) Cohen; J Org Chem 1977, V42(12) CAPLUS  
 (7) Ganushchak; 1992, V28(3), P531 CAPLUS  
 (8) Gutcho; US 2820780 1958 CAPLUS  
 (9) Krauss; US 4734527 1988 CAPLUS  
 (10) Laufer; US 3479407 1969 CAPLUS  
 (11) Ungnade; Org Synth Coll 1955, V3, P130  
 (12) Watson; J Chem Soc 1922, V121, P2414 CAPLUS  
 (13) Werner; US 2286701 1942 CAPLUS  
 (14) Yiannios; J Org Chem 1963, V28, P3246 CAPLUS

## DISPLAY IALL (GTEXT=ON) (cont'd)

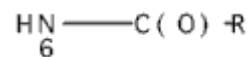
MSTR 1



G1 = arylene (opt. substd.) / 4-1 5-3 / heterocycle <1-10 rings> /  
(specifically claimed phenylene (opt. substd. by G4))



G2 = carbon chain (opt. substd.)  
G3 = arylene (opt. substd.)  
G4 = alkyl / aryl /  
alkyl (substd. by 1 or more aryl)  
/ 6 / alkoxy / NH2 (substd.)



Patent location: claim 3

**MARPAT****DISPLAY FBIB MSTR(1) (GTEXT=ON)**

AN 130:146287 MARPAT  
 TI Liquid crystal composition for display device  
 IN Kaneko, Masaharu; Kadowaki, Masami; Sato, Hideki  
 PA Mitsubishi Chemical Corporation, Japan  
 SO U.S., 16 pp.  
 CODEN: USXXAM

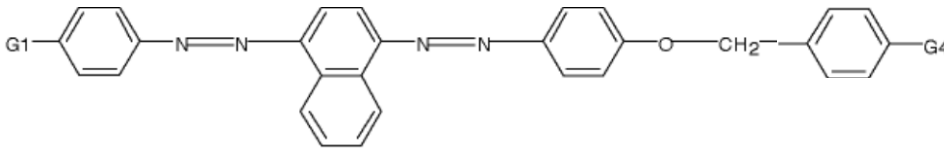
DT Patent  
 LA English  
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	US 5866033	A	19990202	US 97-946859	19971008
				JP 96-277789	19961021
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	JP 10183121	A2	19980714	JP 97-77234	19970328
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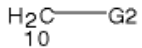
## PATENT FAMILY INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	JP 10183121	A2	19980714	JP 97-77234	19970328
				JP 96-277789	19961021
	US 5866033	A	19990202	US 97-946859	19971008
				JP 96-277789	19961021
				JP 97-27684	19970212
				JP 97-77234	19970328

## MSTR 1



G1 = H / alkyl / alkoxy /  
 alkyl (substd. by alkoxy)  
 / halo / cyclohexyl (opt. substd. by 1 or more G3) /  
 Ph (opt. substd. by 1 or more G3) / 10 / (Examples: octyl / Bu-n)



G2 = cyclohexyl (opt. substd. by 1 or more G3) / Ph (opt. substd. by 1 or more G3)

G3 = alkyl / alkoxy /  
 alkyl (substd. by alkoxy / alkoxy /  
 alkyl (substd. by alkoxy) / halo  
 / cyclohexyl (opt. substd. by 1 or more G3) /  
 Ph (opt. substd. by 1 or more G3) / 39 / (Example: 41)



G5 = heptyl / pentyl / Bu-n

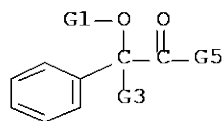
Patent location: claim 1

Note: total number of carbon atoms in alkyl groups substituted with  
 alkoxy groups in G1, G3, and G4 is 2-12

RE.CNT: 4            THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

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

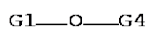
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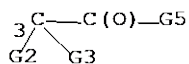
Patent location: claim 1  
 Note: also incorporates claim 10  
 Note: or pharmaceutically acceptable salts, solvates, or prodrugs  
 Stereochemistry: or diastereomers or enantiomers or stereoisomers

## DISPLAY QHIT (SET MPTASSEMBLY OFF)

## MSTR 1



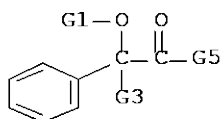
G2 = Ph  
 G4 = 3



Patent location: claim 1  
 Note: also incorporates claim 10  
 Note: or pharmaceutically acceptable salts, solvates, or prodrugs  
 Stereochemistry: or diastereomers or enantiomers or stereoisomers

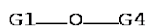
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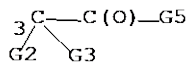


Patent location: claim 1  
 Note: also incorporates claim 10  
 Note: or pharmaceutically acceptable salts, solvates, or prodrugs  
 Stereochemistry: or diastereomers or enantiomers or stereoisomers

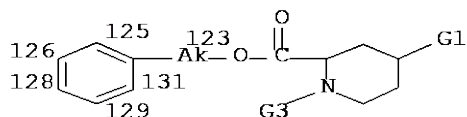
## MSTR 1



G2 = Ph  
 G4 = 3



Patent location: claim 1  
 Note: also incorporates claim 10  
 Note: or pharmaceutically acceptable salts, solvates, or prodrugs  
 Stereochemistry: or diastereomers or enantiomers or stereoisomers

**MARPAT****DISPLAY QHITEXG****MSTR 2 Assembled**

123: alkylene <containing 1-4 C>  
 125, 126, 128, 129, 131: opt. substd. by G7

## Additional displayed G-groups:

G1 = alkyl <containing 1-10 C> /  
 any ring <containing zero or more N, zero or more O,  
 zero or more S (no other heteroatoms), aromatic, 1-3 rings,  
 including 5- or 6-membered rings> (opt. substd. by G7) /  
 (Specifically claimed: Me / Ph (opt. substd. by G7)) /  
 (Examples: Et / Pr-n / Pr-i / Bu-n / Bu-i / Bu-s / Bu-t)

G3 = H / R

Patent location: claim 6  
 Note: also incorporates claim 7  
 Note: or salts

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