Markush Search Report

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Markush Structure

Markush structures is a generic structure which can represent lot of specific structures. The generic structures are prepared with lot of variations like:

- R-groups (substituent variation)
- Atom, bond lists
- Repeating units (link nodes and groups)
- Position variation (variable point of attachment)
- Homology variation (e.g. alkyl, aryl)
- Conditions for generic features: occurrence lists, dependency, etc

Like this report?

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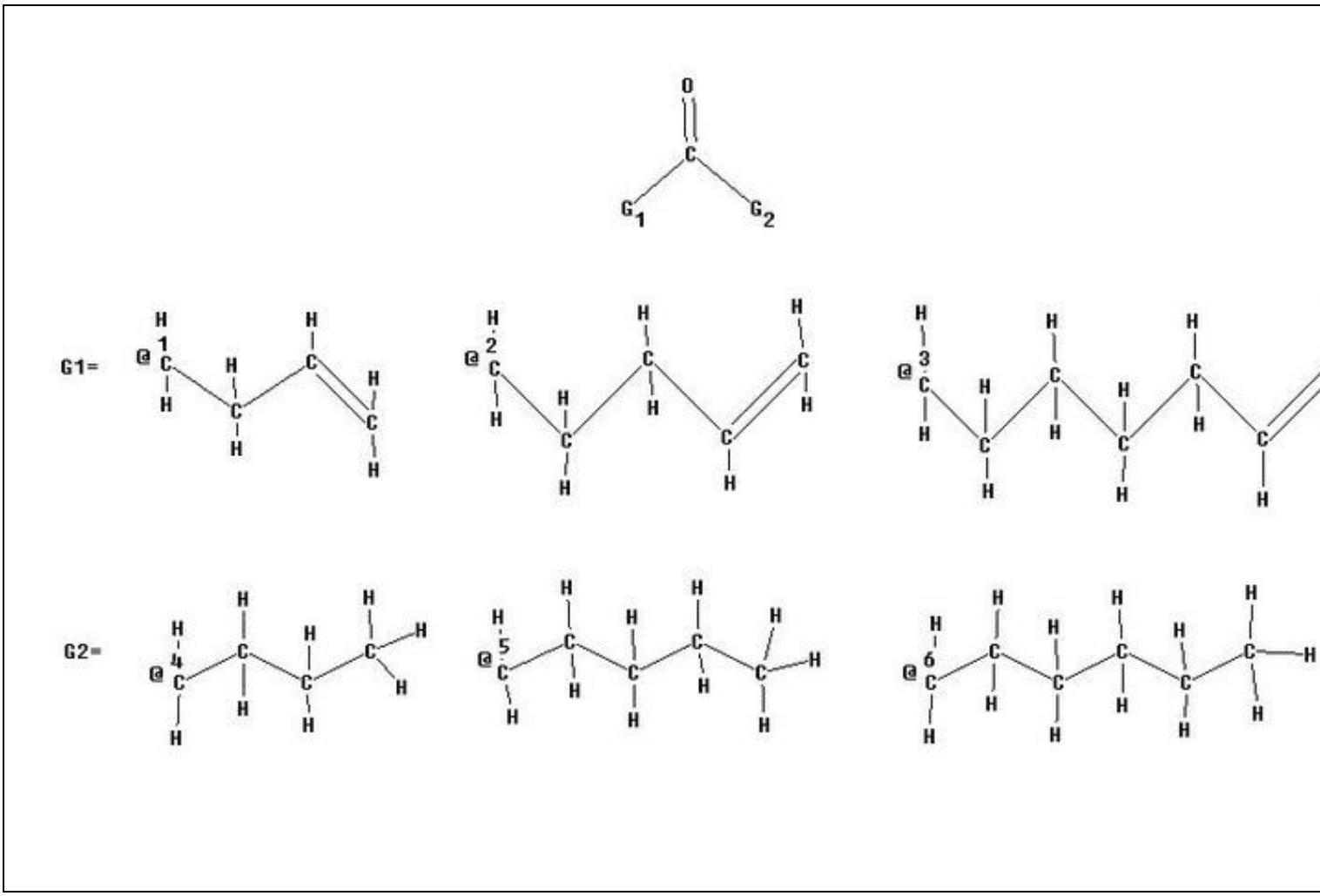
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Demonstration of a Markush Structure Search

The specific structures are

- Undec-1-ene-5-one
- Dec-1-ene-6-one
- Undec-1-ene-7-one

These specific structures are represented by using one markush structure. And it is



Alkenone

Search Transcript

The following query is search done for above markush structure:

=> FILE CASLINK

COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 0.22 0.22

FILE 'CAPLUS' ENTERED AT 07:55:57 ON 26 JUN 2009
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CLUSTER 'CASLINK' ENTERED

Predefined command sequences will be executed in REGISTRY, MARPAT, and CAPLUS.

=> Uploading C:\Documents and Settings\naveenm\My Documents\STN Express 8.4\Queries\alcohols.str

L1 structure uploaded

=> D L1

=> S L1 SSS SAM

S L1 SSS SAM FILE=REGISTRY
SAMPLE SEARCH INITIATED 07:57:24 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 85742 TO ITERATE

2.3% PROCESSED 2000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1697409 TO 1732271
PROJECTED ANSWERS: 60071 TO 66827

L2 50 SEA SSS SAM L1
PLE SCREEN SEARCH COMPLETED-16196 TO ITERATE

=> D SCAN

L3 50 ANSWERS MARPAT COPYRIGHT 2009 ACS on STN
CC 5-6 (Agrochemical Bioregulators) TI Halo substituted aryloxyalkylimidazolines for use as pesticides ST halo aryloxyalkylimidazoline deriv insecticide nematicide molluscicide IT Blattaria, Coleoptera, Diptera, Heliothis virescens, Hemiptera, Hymenoptera, Insecticides, Isoptera, Lepidoptera, Molluscicides, Myzus persicae, Nematocides, Orthoptera, Siphonaptera, Thysanoptera

MSTR 1

G15 = alkenyl <containing 2-10 C> (opt. substd.)
G17 = 21 / 32 / 42
G19 = 34

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> S L1 SSS FULL

S L1 SSS FUL FILE=REGISTRY
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:Y
FULL SEARCH INITIATED 07:58:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1714320 TO ITERATE
92.0% PROCESSED 1576643 ITERATIONS 73014 ANSWERS
100.0% PROCESSED 1714320 ITERATIONS 73119 ANSWERS
SEARCH TIME: 00.00.27

L3 73119 SEA SSS FUL L1

SET PLURAL ON PERM
SET ABBREVIATION L ON PERM
SET SPELLINGS ON PERM

=> S biofilm OR (polymeric(W)film) OR (polymer?(3A)dispersion?)

S BIOFILM OR (POLYMERIC(W)FILM) OR (POLYMER?(3A)DISPERSION?) FILE=CAPLUS
L4 50796 FILE CAPLUS
1 FILES SEARCHED...

=> S calculus OR tartar? OR plaque?

S CALCULUS OR TARTAR? OR PLAQUE? FILE=CAPLUS
L5 107110 FILE CAPLUS
1 FILES SEARCHED...

=> S (oral(W)disinfect?) OR decoloni? OR (anti(W)bacterial) OR reduc?(3A)bacter?

S (ORAL(W)DISINFECT?) OR DECOLONI? OR (ANTI(W)BACTERIAL) OR REDUC?(3A)BACTER? FILE=CAPLUS
L6 25142 FILE CAPLUS
1 FILES SEARCHED...

=> S malodo##### OR odorifer? OR (bad(W)breath) OR (breath (A) fresh?)

S MALODO##### OR ODORIFER? OR (BAD(W)BREATH) OR (BREATH (A) FRESH?) FILE=CAPLUS
L7 9031 FILE CAPLUS
1 FILES SEARCHED...

=> S Periodon? OR Dent###### OR (mouth(W)care) OR (mouth(W)wash) OR (mouth(W)rinse)

S PERIODON? OR DENT###### OR (MOUTH(W)CARE) OR (MOUTH(W)WASH) OR (MOUTH(W)RINSE) FILE=CAPLUS
L8 101339 FILE CAPLUS
1 FILES SEARCHED...

=> S L3 AND L4

S L3 AND L4 FILE=CAPLUS
L9 3093 FILE CAPLUS
1 FILES SEARCHED...

=> S L3 AND L5

S L3 AND L5 FILE=CAPLUS
L10 2 FILE CAPLUS
1 FILES SEARCHED...

=> S L3 AND L6

S L3 AND L6 FILE=MARPAT
L11 462 FILE MARPAT
1 FILES SEARCHED...

=> S L3 AND L7

S L3 AND L7 FILE=CAPLUS
L12 3093 FILE CAPLUS
1 FILES SEARCHED...

=> S L3 AND L8

S L3 OR L8 FILE=CAPLUS
L13 3095 FILE CAPLUS
1 FILES SEARCHED...

=> S L9 OR L10 OR L11 OR L12 OR L13

S L9 OR L10 OR L11 OR L12 OR L13 FILE=CAPLUS
L14 3511 FILE CAPLUS
1 FILES SEARCHED...

=> S A61K0007-16/IPC OR A61K0007-30/IPC OR A61Q0011-00/IPC

L15 101339 FILE CAPLUS
1 FILES SEARCHED...
=> S (L14 AND L15)

L16 1960 (L14 AND L15)

=> S L16 AND PATENT/DT

L17 1000 L16 AND PATENT/DT

=> D L17 IALL 1

L17 ANSWER 1 OF 1000 MARPAT COPYRIGHT 2009 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 132:255813 MARPAT Full-text
TITLE: Dental surface coating agents and oral compositions containing the dental surface coating agents
INVENTOR(S): Segawa, Hiroyuki; Okano, Ryuji; Naito, Junko
PATENT ASSIGNEE(S): Earth Chemical Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp. CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
INT. PATENT CLASSIF.:
MAIN: A61K007-16
SECONDARY: A61K006-00
CLASSIFICATION: 62-7 (Essential Oils and Cosmetics)
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 2000103726 A 20000411 JP 1998-278254 19980930
JP 3909787 B2 20070425
PRIORITY APPLN. INFO.: JP 1998-278254 19980930
ABSTRACT:
Fatty acid salts as dental surface coating agents and oral compns. containing the dental surface coating agents are claimed. An oral composition contained CPC 0.01, sodium oleate 0.2, glycerin 15, POE/POP block copolymer 0.2, phosphoric acid salts 0.5, flavors 1.0 g, denatured alc. 5 mL and appropriate amount of purified water.

SUPPL. TERM: dental surface coating fatty acid salt; sodium oleate dental surface coating dentifrice
INDEX TERM: Dentifrices Mouthwashes (dental surface coating agents and oral compns. containing the dental surface coating agents)
INDEX TERM: Tooth (dental surface coating agents; dental surface coating agents and oral compns. containing the dental surface coating agents)
INDEX TERM: 143-19-1, Sodium oleate
ROLE: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses) (dental surface coating agents and oral compns. containing the dental surface coating agents)

MSTR 1

G1= alkenyl<containing 9-19 C> / (Examples: 4 / 10 / 14 / 19)

G2= Na / K / NH3
Patent location: claim 1

=> LOGOFF Y

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