

Index Chemicus®

FILE DESCRIPTION

Index Chemicus focuses on current awareness of new compounds and reports with over 200,000 new compounds and synthetic intermediates added each year, with coverage of over 2.4 million structures published in the literature since 1993. Covering the world's leading organic chemistry journals, *Index Chemicus* is a text- and substructure-searchable database. It serves as both a compound database and a current awareness tool, providing full graphical summaries, complete bibliographic information, and author abstracts for the papers it covers.

With *Index Chemicus*, a user can:

- keep up with the latest research
- find new ideas for projects
- track the work of other research groups
- save time in the laboratory and the library

SUBJECT COVERAGE

Index Chemicus (File 302) contains the structures and critical supporting data for novel organic compounds reported in over 100 leading international journals. In addition, many full records in the database show the reaction flow from starting material to final product. *Index Chemicus* is a vital source of new information on biologically active compounds and natural products.

TIPS

USE FILE 302

to keep up on the latest chemical research activities taking place worldwide.

S METH(W)OXY AND TRANSFERASE

USE DialogLink™ 5 and FILE 302

to graphically search and display the chemical structures within *Index Chemicus*.

USE CORPORATE SOURCE (CS=)

to track the work of other research groups

S CS=(ARIZONA(W)STATE)

USE BA= and MAP BA

to search for biologically active compounds and then save the biological activity terms for further searching in other files.

S BA=TRYPSIN INHIBITING?

MAP BA TEMP S3

DIALOG FILE DATA

Inclusive Dates: 1993 forward

Update Frequency:

Weekly 4,000 new compounds added per update
from 325 articles

File Size:

2.4 Million compounds from 202,000 records as of
November 1, 2005

CONTACT

Index Chemicus is produced by Thomson Scientific, Inc. Questions concerning file content should be directed to:

Thomson Scientific, Inc.

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SAMPLE RECORD

DIALOG(R)File 302:INDEX CHEMICUS
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0000179426

/TI **Total-synthesis and in-vitro-antifungal activity of (+/-)-2-methoxytetradecanoic acid**

AU= **Author(s):** Carballeira NM; Ortiz D; Parang K; Sardari S

CS= **Corporate Source:** Univ Puerto Rico, Dept Chem, San Juan, PR 00931 USA;
Univ Rhode Isl, Coll Pharm, Dept Biomed Sci, Kingston, RI 02881 USA

JN=,SN= **Journal Name:** ARCHIV DER PHARMAZIE 337 (3): 152-155 **ISSN:** 0365-6233
Item Count: 0007

PD=,PY= **Publication Date:** MAR, 2004 (20040300)

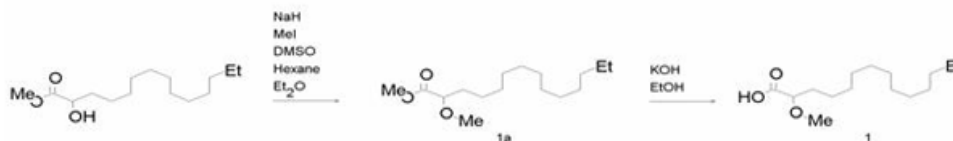
DT=,RT= **Document Type:** Journal **Record Type:** Article

LA= **Language:** English

PU= **Publisher:** WILEY-V C H VERLAG GMBH, PO BOX 10 11 61, D-69451

WEINHEIM, GERMANY. JOURNALS ADMINISTRATION DEPT. 1 OLDLANDS WAYS BOGNOR
REGIS, W SUSSEX PO 22 9SA, ENGLAND.

Structure Image or Graphical Abstract Diagram



/AB **Abstract:** The marine fatty acid (+/-)-2-methoxytetradecanoic acid was synthesized in two steps (71% overall yield) starting from commercially available methyl-2-hydroxytetradecanoate. The title compound was antifungal against *Candida albicans* (ATCC 14053) in RPMI medium and *Aspergillus niger* (ATCC 16404) and *Cryptococcus neoformans* (ATCC 66031) in SDB medium at the minimum inhibitory concentration (MIC) of 100 mM, which compares to the fungitoxicity of a 2-iodotetradecanoic acid against the same fungi. The title compound was also five to ten times more cytotoxic than capric acid to *C. albicans* and *A. niger* in the tested medium but comparable in cytotoxicity to either capric acid and its 2-methoxylated analog to *C. neoformans*. The antifungal activity of (+/-)-2-methoxytetradecanoic acid is explained in terms of inhibition of N-myristoyltransferase.

/DE **Descriptors:**

KeyWords Plus: CANDIDA-ALBICANS; FATTY-ACIDS

Keywords (Author): 2-METHOXYTETRADECANOIC ACID; MYRISTIC ACID;
ANTIFUNGAL ACTIVITY; N-MYRISTOYLTRANSFERASE

NC= **No. of Compounds:** 2

Compound Number: 670205001

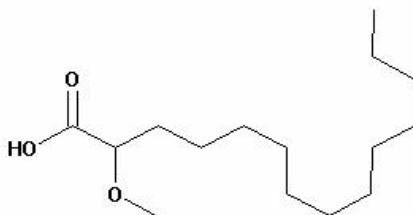
Compound ID: 1

/DE,BA= **Bioactivity--Activity Status:**

ANTIFUNGAL ACTIVITY--Tested

ENZYME INHIBITING ACTIVITY--Tested

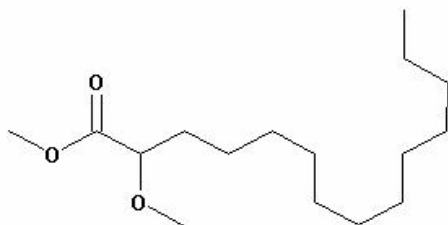
TRANSFERASE INHIBITING ACTIVITY--Tested



[Edit Molecule]

SAMPLE RECORD (cont'd)

Compound Number: 670205002
 Compound ID: 1a



[Edit Molecule]

SEARCH OPTIONS

BASIC INDEX

| SEARCH SUFFIX | DISPLAY CODE | FIELD NAME | INDEXING | SELECT EXAMPLES |
|---------------|--------------|--|-------------------------|--|
| — | — | All Basic Index Fields | Word | S METH(W)OXY S STRUCTUR?(W)ANALYSIS |
| /AB | AB | Abstract ¹ | Segment & Word | S METH(W)OXY/AB S TUMOR(W)CELL?/AB S METHOXY/FW |
| /DE | DE | Descriptor ^{1,2,3,4} | Segment & Word & Phrase | S METH(W)OXY/DE S MYRISTIC(W)ACID/DE S N-MYRISTOYLTRANSFERASE/DE S CANDIDA/DF |
| /SY | SY | Trivial Chemical Name (Synonym) ^{1,4} | Segment & Word & Phrase | S METH(W)OXY/SY S CYCLOHEXANE/SY S PHE-GLY-ASN?/SY S ARG(S)TYR/SY |
| /TI | TI | Title ¹ | Segment & Word | S TOTAL(W)SYNTHESIS/TI S AZO(W)DI/TI |

¹ The chemical names (common or systematic) are indexed as chemically significant segments, individual words and complete phrases, depending on the indexing of the field the name is found in. Use /FW, Full Word, to limit to the unsegmented term.

² Includes Bioactivity terms, KeyWords Plus and Author Keywords.

³ Also searchable using /DF

⁴ Searchable in the Basic Index and Additional Indexes.

ADDITIONAL INDEXES

| SEARCH PREFIX | DISPLAY CODE | FIELD NAME | INDEXING | SELECT EXAMPLES |
|-----------------|----------------|--|--|---|
| AU= — BA= | AU AZ BA | Author Name DIALOG Accession Number Biological Activity ⁴ | Phrase Word & Phrase Word & Phrase Phrase | S AU=CARBALLEIRA NM S BA=TRANSFERASE INHIBITING ACTIVITY S BA=(TRYPSIN(W)INHIBITING) S CS=(ARIZONA(W)STATE) S CS=ARIZONA STATE? S DT=JOURNAL |
| CS= | CS | Corporate Source | | |
| DT= | DT | Document Type | | |
| — | GR | Grade ⁵ | | |
| — | GS | Searchable Chemical Structure | | |
| — | IM | Structure Image or Graphical Abstract Diagram | | |
| JN= | JN | Journal Name | Phrase | S JN=ARCHIV DER PHARMAZIE |
| LA= | LA | Language | Phrase | S LA=ENGLISH |
| NA= | NA | Trivial Chemical Name (Synonym) ⁴ | Phrase | S NA=2-DEACETYLTAXINE A S NA=ALA-LEU-ALA? S NA=CUPANIOL |
| NC= | NC | Number of Compounds ⁷ | Phrase | S NC=02 |
| — | OT | Original Article Title | | |
| PD= | PD | Publication Date | Phrase | S PD=20040300 |
| PU= | PU | Publisher Name | Phrase | S PU=WILEY V C H? |
| PY= | PY | Publication Year | Phrase | S PY=2004 |
| RT= | RT | Record Type | Phrase | S RT=ARTICLE |
| SN= | SN | ISSN | Phrase | S SN=0365-6233 |
| — | SO | Journal Source Information ⁶ | | |
| ST= | ST | Status of Bioactivity Testing | Phrase | ST=TESTED ST=POTENTIAL |
| SY= | SY | Trivial Chemical Name (Synonym) ⁴ | Phrase | S SY=ALA-ASP-? S SY=CUPANIOL |

⁵ The graphic structure can be displayed using DialogLink 5. All other interfaces currently display the text equivalent of the .MOL file. The GS display code can be combined with any user-defined format or any pre-defined format, except format 1.

⁶ SO (journal source information) includes the journal name, volume, issue, pages, ISSN and publication date.

⁷ Compound Number is the sequential number within Index Chemicus and Compound ID is the compound reference number used by the author

SPECIAL FEATURES

For command descriptions, enter HELP LIMIT, HELP SORT, HELP RANK, HELP MAP, HELP DUP online.

| | | |
|---------------|--|--|
| SORT | AU, JN, PD, PY, TI | SORT S6/ALL/TI |
| RANK | All phrase- and numeric-indexed fields in the Additional Indexes can be ranked. Other RANK codes include: DE | RANK DE RANK NA S4 RANK JN S8/1-34 |
| MAP | BA, NA, SY | MAP BA TEMP S1 |
| RD, ID | Remove duplicates (RD) or identify duplicates (ID,IDO). | RD S5 |

PREDEFINED FORMAT OPTIONS

| NO. | DIALOGWEB FORMAT | RECORD CONTENT |
|-----|---------------------|--|
| 1 | -- | DIALOG Accession Number |
| 2 | -- | Full Record, except abstract |
| 3 | Medium | Dialog Accession Number, Item Count, Number of Compounds, Title, Journal Name, Author, Corporate Source, Publisher, Language and Trivial Chemical Name |
| 4 | -- | Full Record - tagged |
| 5 | Long | Full Record |
| 6 | -- | Dialog Accession Number, Item Count, Number of Compounds and Title |
| 7 | -- | Full Record |
| 8 | Short | Dialog Accession Number, Item Count, Number of Compounds, Title, KeyWords Plus and Author Keywords |
| 9 | Full | Full Record |
| 19 | -- | Full Record |
| K | -- | KWIC (Key Word In Context) displays a window of text; may be used alone or with other formats |

OTHER OUTPUT OPTIONS

For an explanation, enter HELP TYPE, HELP UDF, HELP TAG online.

| | | |
|-----------------------------|---|--|
| USER DEFINED FORMATS | Display codes listed in the Search Options tables can be used to customize output. | TYPE S4/JN,SY/ALL |
| TAG | Output can be displayed with tags identifying each display field. | TYPE S3/3/1-5 TAG |
| DIRECT RECORD ACCESS | If the accession number of a specific record is known, it can be used to display the record directly. | TYPE 0179426/9 DISPLAY 0179426/TI,AU PRINT 0179426/3 |

FOR ONLINE HELP:

See HELP FIELDS 302 for searchable fields; HELP FORMAT 302 for output formats; HELP LIMIT 302 for limits; HELP RATES 302 for cost information; HELP SORT 302 for sorts.