

Introduction

The *Handbook of Active Marine Natural Products* covers eight volumes. This book is *Volume 1: Terpenoids, Part 1*, which includes 1,131 active compounds.

Format of Compound Entry. A compound entry starts with a title line, which has two items: the compound's unique code (from 1 to 1,131 for volume 1) and the main name. The following eight items form the title line as a body, and the graphic structure is placed at the end:

Title line (code number, main name)

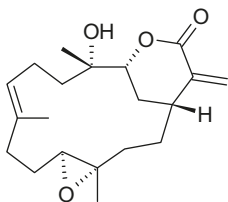
- A. Synonyms of the compound (if any)
- B. Structural type
- C. Formula (relative molecular mass)
- D. Physicochemical properties
- E. Marine source(s)
- F. Pharmacological data (if any)
- G. Reference(s)
- Graphic structure

Chemical Names and A. Synonyms. Generally, a compound may have one scientific name and several trivial names. In the handbooks, based on original articles, we select one name as the "main name." The main name appeared at the title line of each compound entry. In most cases, a trivial name was selected as the main name, and in some cases, the main name is a scientific name. Any synonyms, if any, are presented after the title line as an item A of the entry body.

B. Structural Type. Structural type is the second item, ordered by the contents order.

F. Normalization of Pharmacological Data. All of 1,131 MNP components in this book have pharmacological data, which are very valuable. Because different expressions are used for the same kind of data in different articles, we have to define and normalize thousands of pharmacological terms, so that the data could be expressed in a unified way, and be easily understood by readers.

Stereochemistry in Graphic Structure. We protracted all compound structures down to atomic bond level, including complicated glycosides, with stereochemical information based on the data in the original papers. For example, the structure with full stereochemistry of the compound 730 sinularin is



Let us further explain the data structure of source terms and pharmacological terms.

Source Terms

The source data of the compound 730 sinularin is

Source:

Soft coral *Sinularia* sp. (Dongluo I. Hainan, South China Sea)

Soft coral *Sinularia triangula* (Taitung County, Taiwan)

Soft coral *Sinularia flexibilis*

Soft coral *Sinularia capillosa*

The format is as follows (banding the English-type name and the Latin name together):

Source:

English-type name + Latin name of source 1 (sampling place, sampling season water depth, etc., if any)

English-type name + Latin name of source 2

English-type name + Latin name of source 3

English-type name + Latin name of source 4

Pharmacological Terms

The pharmacological terms in the handbooks are presented in a multilayered structure. In the top layer, there are more than 20 types of the most important pharmacological activity terms. They are cytotoxic (*in vitro* anticancer), antineoplastic (*in vivo* anticancer), antibacterial, antifungal, antiviral, anti-HIV, anti-inflammatory, antioxidant, antimalarial, NO (nitric oxide) production inhibitors, enzyme inhibitors, cardiovascular activity, smooth muscle relaxant and stimulant, toxin and medium lethal dose (LD₅₀), and so forth. Readers need to be familiar with these Tope lever pharmacological terms (see Table 1).

For each term there is a regulation about how to describe related pharmacological data. The following is an example. Under the subtitle “Pharm:” of the compound 730 Sinularin, a set of multiple biodata is presented as follows:

Pharm:

Cytotoxic (CCRF-CEM, ED₅₀ = 26.0 μmol/L, control doxorubicin, ED₅₀ = 0.57 μmol/L, DLD-1, ED₅₀ = 37.1 μmol/L, doxorubicin, ED₅₀ = 0.25 μmol/L);

anti-inflammatory [immunoblot analysis assay, 10 μmol/L, RAW264.7 macrophage cells, inhibition of LPS-induced upregulation of iNOS and COX-2, reduced COX-2 to ≈ 85%, reduced iNOS to (1.2 ± 0.3)%];

Table 1: Twenty-Four Main Pharmacological Terms in Tope Lever.

Order in Index 5	Pharmacological Terms in Tope Lever
1	Anti-AD
2	Antibacterial
3	Antifungal
4	Anti-HIV
5	Anti-inflammatory
6	Antileishmanial
7	Antimalarial
8	Antineoplastic (in vivo)
9	Antioxidant
10	Antiplasmodial
11	Antitrypanosomal
12	Antituberculosis
13	Antiviral
14	Cardiovascular activity
15	Cell cycle inhibitor
16	Cell division inhibitor
17	Cell growth inhibitor
18	Cell adhesion inhibitor
19	Cytotoxic (in vitro)
20	Enzyme inhibitors
21	NO production inhibitors
22	Smooth muscle relaxant and stimulant
23	Toxin
24	Medium lethal dose (LD ₅₀)

antibacterial (gram-positive bacteria);

NF-κB inhibitor (cell-based HEK-293 NF-κB luciferase reporter gene assay, IC₅₀ = 5.30 μg/mL; NF-κB plays a key role in regulating immune response to infection, incorrect regulation of NF-κB has been linked to cancer, inflammatory and autoimmune diseases, septic shock, viral infection, and improper immune development).

The format is as follows:

Pharm:

Term name 1 (formatted detail information)

Term name 2 (formatted detail information)

Term name 3 (formatted detail information)

Term name 4 (formatted detail information)

Under the *term name* *Cytotoxic*, a set of multiple cytotoxic biodata is presented as follows:

Cytotoxic

CCRF-CEM, $ED_{50} = 26.0 \mu\text{mol/L}$, control doxorubicin, $ED_{50} = 0.57 \mu\text{mol/L}$,
DLD-1, $ED_{50} = 37.1 \mu\text{mol/L}$, control doxorubicin, $ED_{50} = 0.25 \mu\text{mol/L}$;

The format is as follows:

Term name (*in vitro/in vivo*,
target cancer cell 1, quantitative data,
positive control compound, control's quantitative data (if any);
target cancer cell 2, quantitative data,
positive control compound, control's quantitative data (if any);
brief description of related mechanism if any).

In order to standardize abbreviations of cancer cells, such as P₃₈₈, A549, HT29, MEL28, CCRF-CEM, and DLD-1, we defined and used 438 cancer cell codes (CCC) in the handbooks. For explanations of these codes, please see "List of Cancer Cell Codes."

By means of the formatted and structuralized methods, we have normalized expressions of almost all the pharmacological data discussed in the handbooks. For complete information in volume 1, of all 674 normalized pharmacological activity terms, please see "Index 5 Compound Pharmacological Activity Index."

In summary, these handbooks with eight volumes provide an integrated collection of 8,350 marine natural products' chemical components isolated from 3,025 marine organisms and a large amount of pharmacological activity data of these components. It might be used not only as a handbook to look for structures and bioactivities of marine natural products and marine organisms source information, but also as a fundamental platform for studying the marine natural products with a systematic and integrative approach.

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