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Enhancing the User Experience for Wiley Chemistry Content

Reinhard Neudert

- Introduction

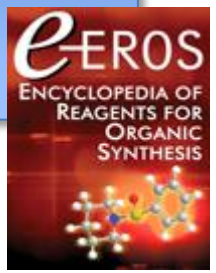
- Chemistry Enrichment Workflow
  - Scheme templates
  - Scheme Enumeration
  - Text Annotation

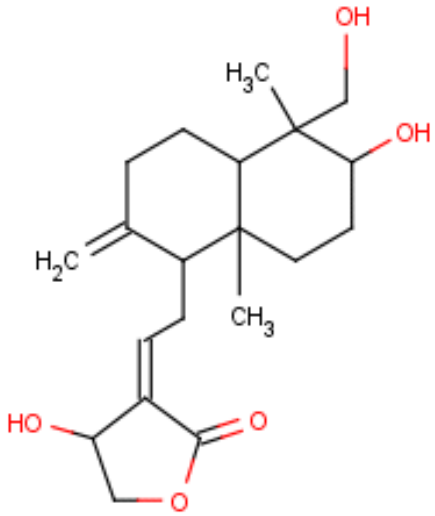
- The Smart Article
  - How to access Smart Articles
  - Navigation in Smart Articles
  - Chemistry Search

Introduction: Discover Wiley Chemistry

Journals

Databases





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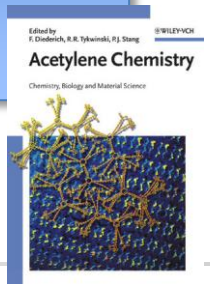
Books



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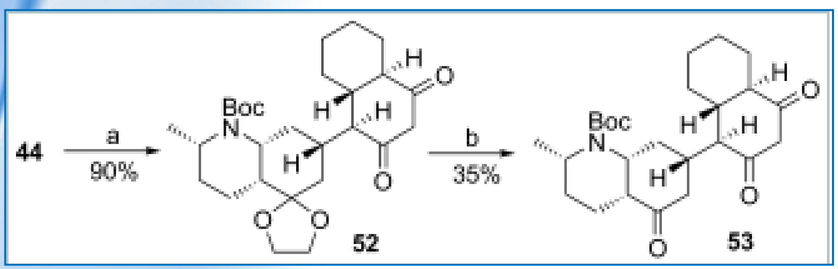
Chemistry in Authors Publications

Challenge!!

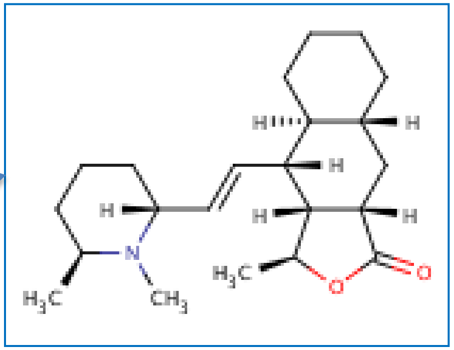
Searchable Compound Repository



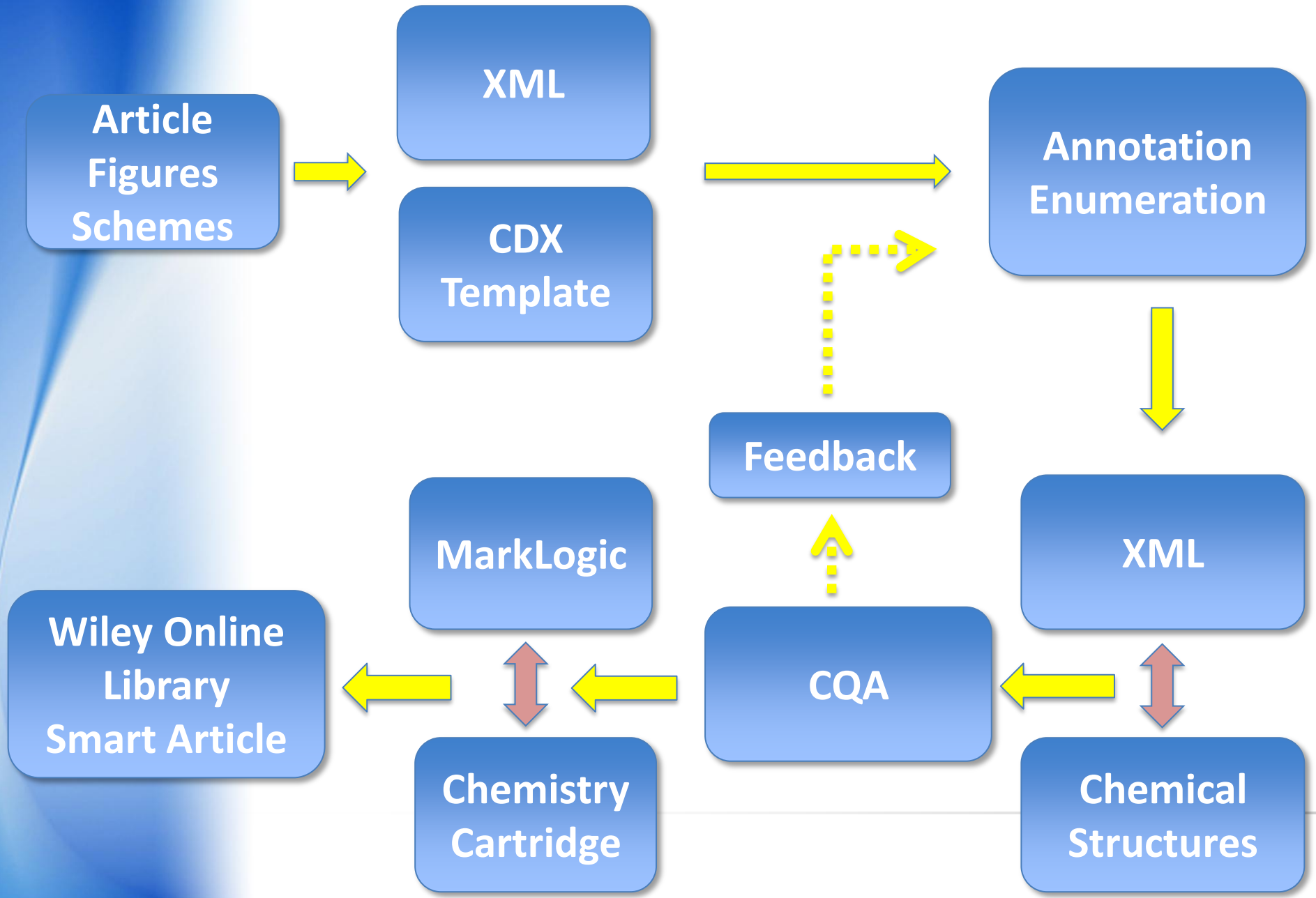
Schemes: CDX (ChemDraw)

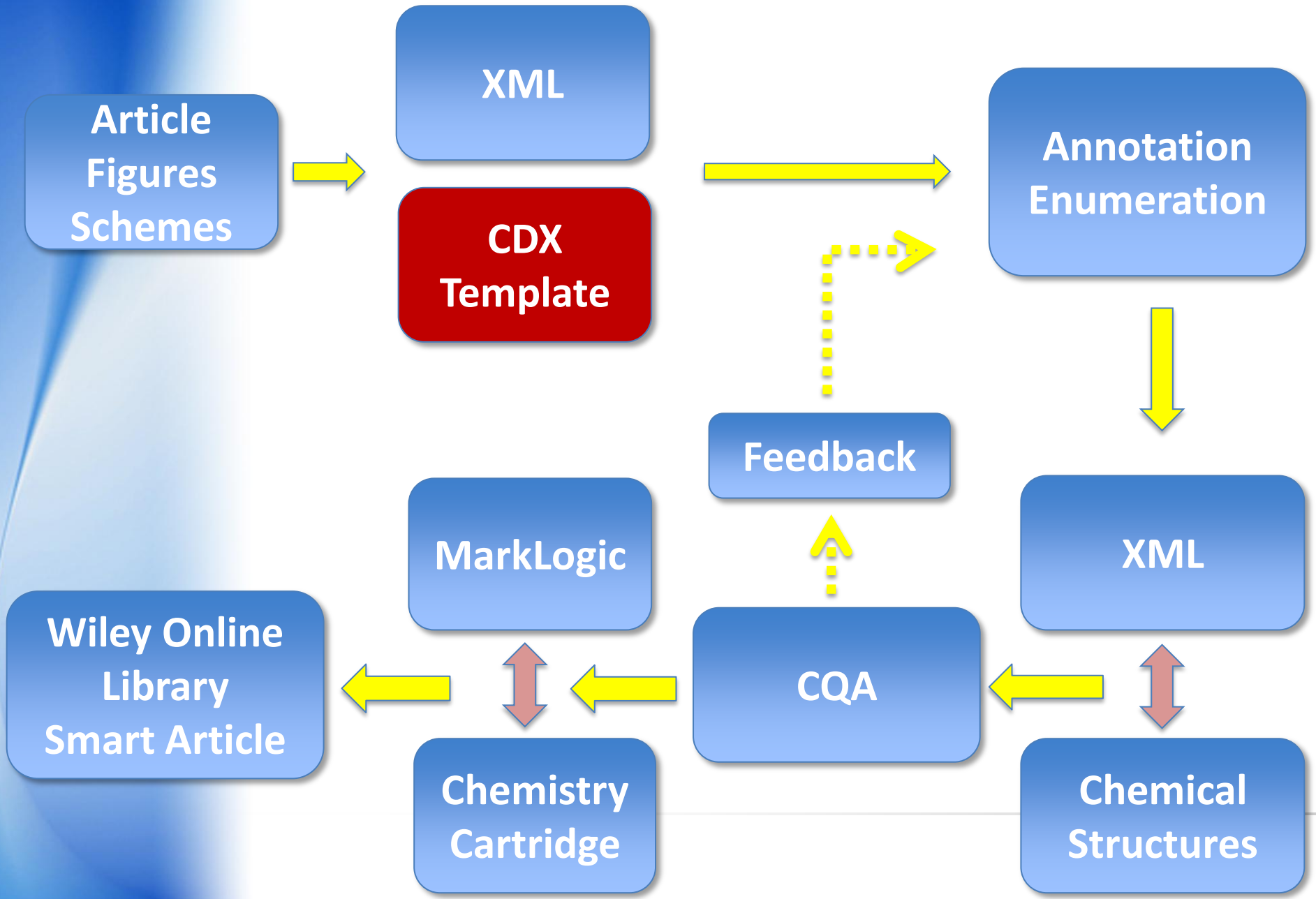
Text

Recently, GB 16 (5),5 a new member of this
attention from the pharmaceutical industry,
and himbacine (1) has shown potent musc



Chemistry Enrichment Workflow

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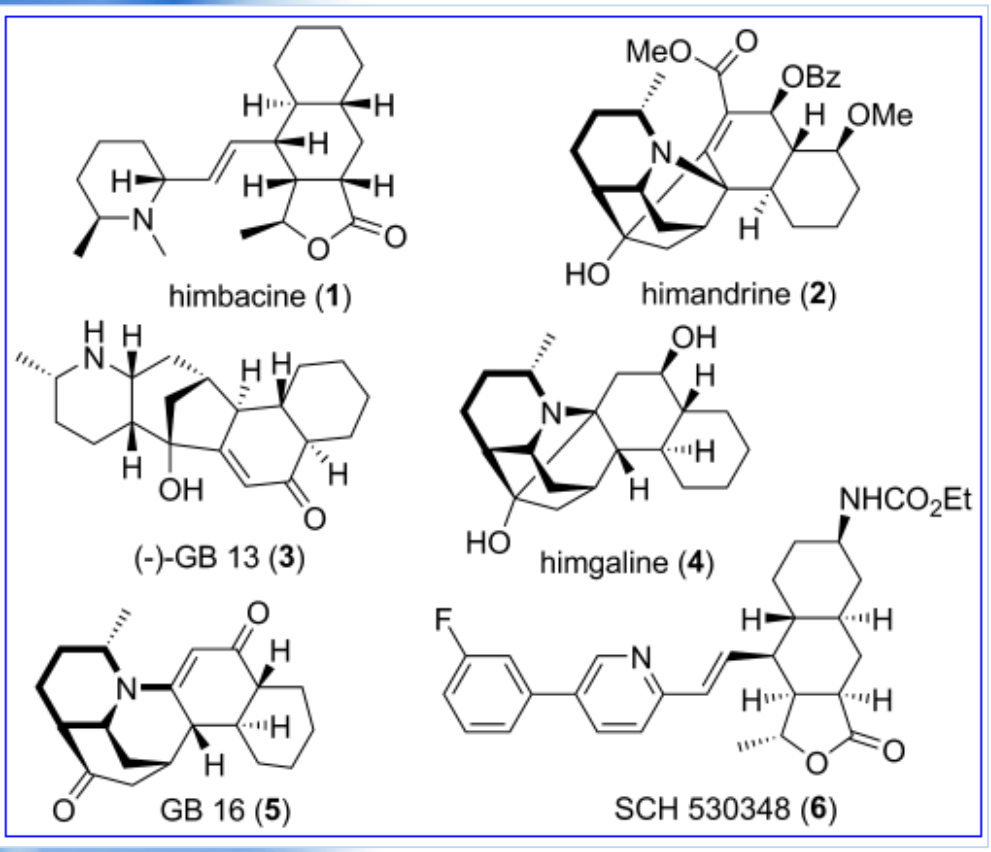
CDX Template: Case1

Author's CDX File



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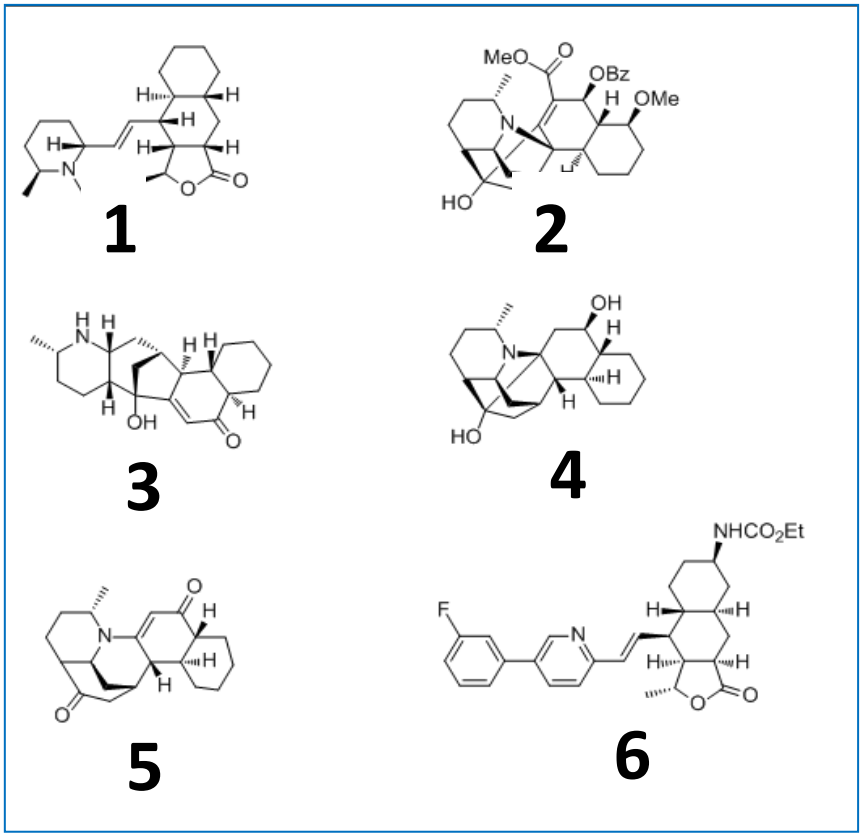
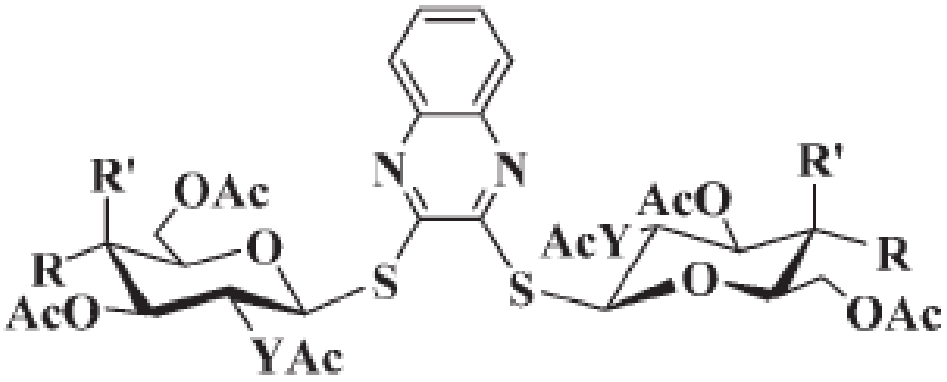


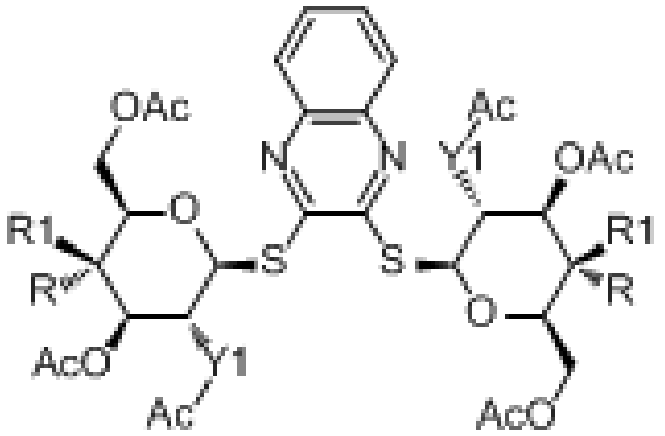
CDX Template: Case2

Author‘s CDX File



5 R = OAc, R' = H, Y = O
6 R = H, R' = OAc, Y = O
7 R = OAc, R' = H, Y = NH

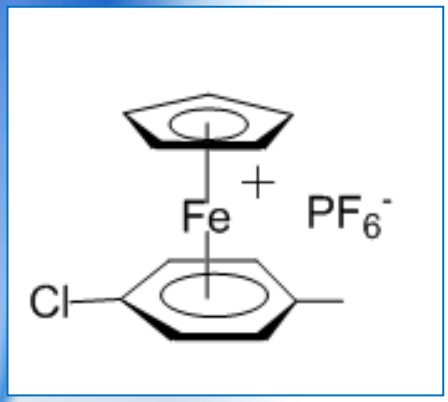
CDX Template

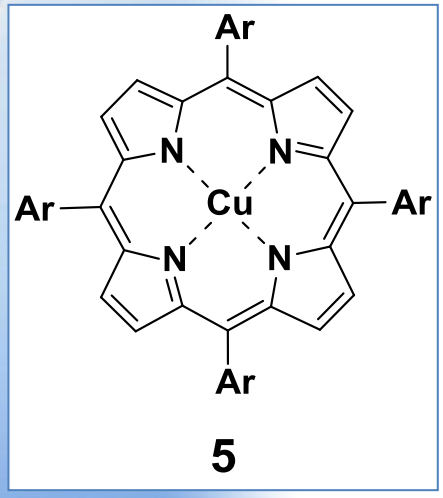


Caption	R	R1	Y1
5	OAc	H	O
6	H	OAc	O
7	OAc	H	NH

CDX Template: more…

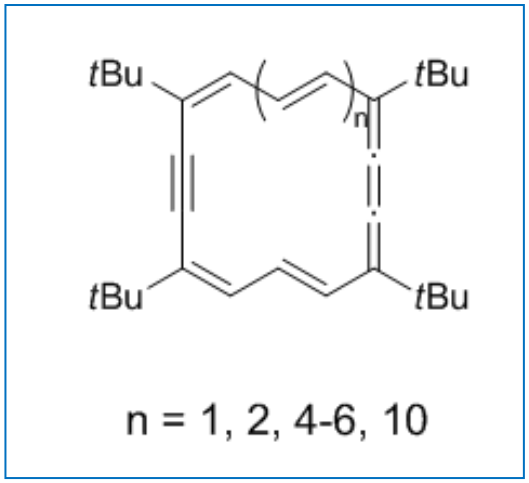
Organometalic Chemistry





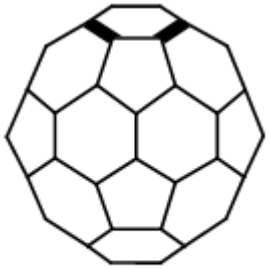
5

Repeating Groups



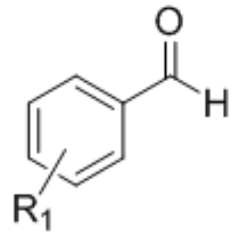
n = 1, 2, 4-6, 10

Planar Fullerens

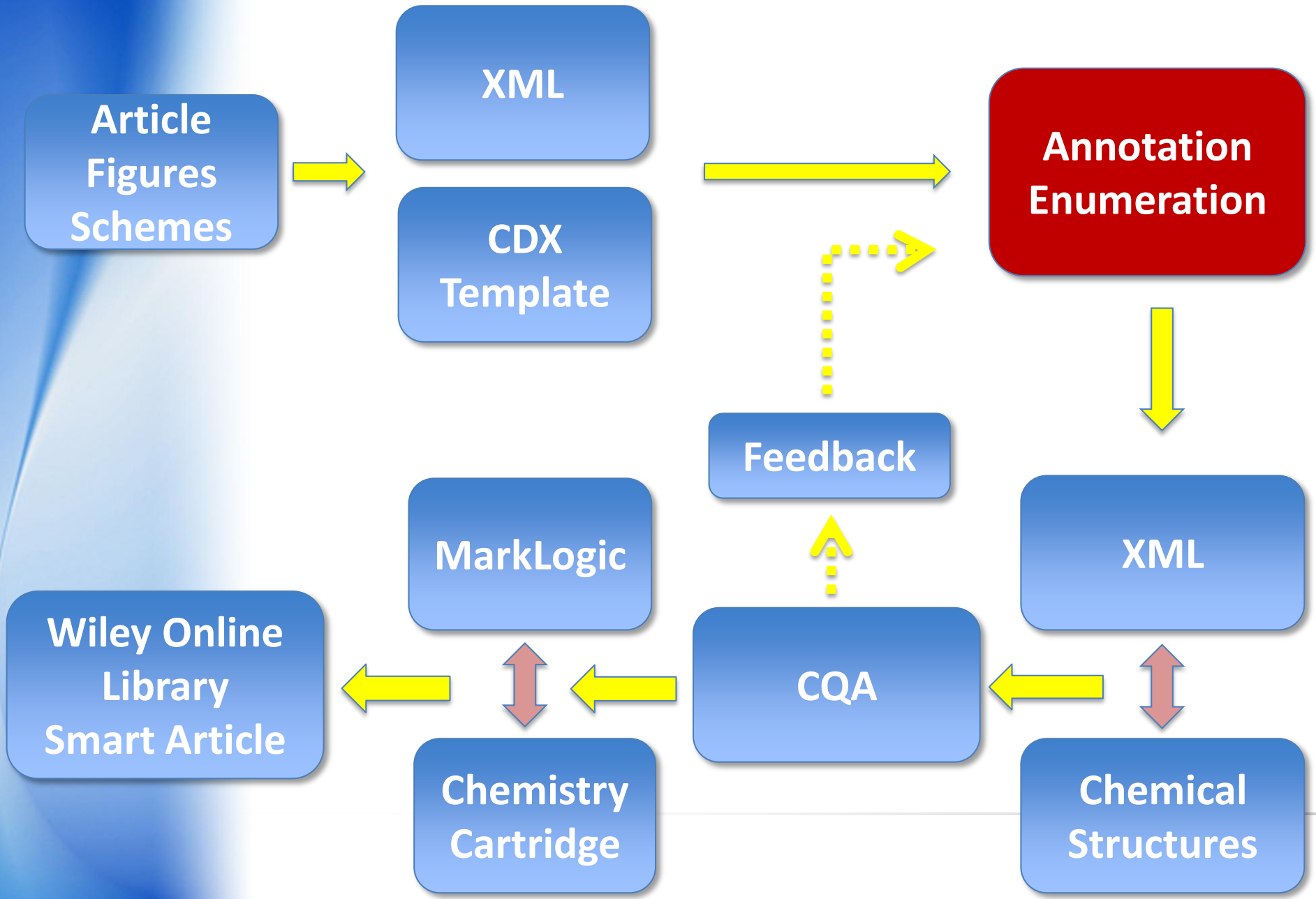


cis-**1** (C_s)

Variable Points of Attachments



R^1 = Me, Et, COOH, 4-MeC_6H_4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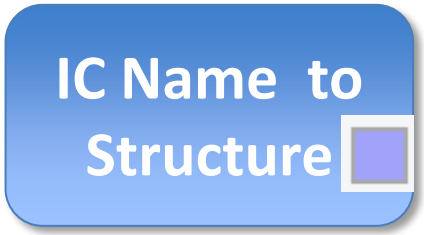
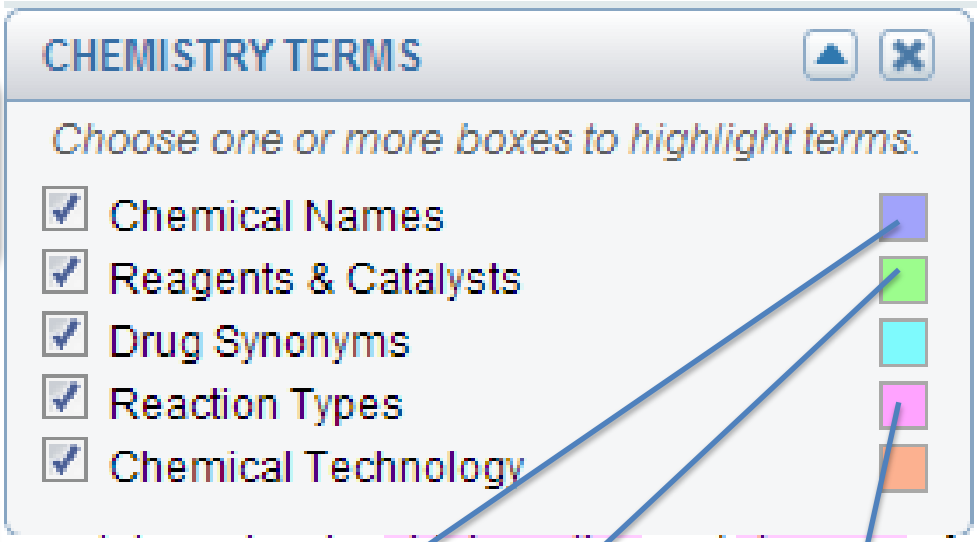
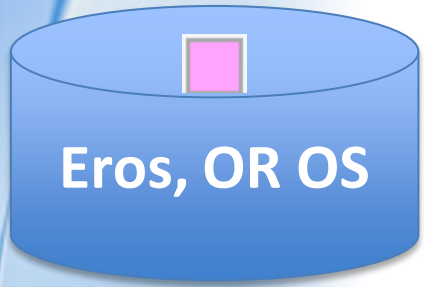
Annotation Enumeration







oxidation19 process as indicated in Scheme 7. After the failed attempt of inhibiting the formation of **46** pyridinium chlorochromate (PCC)17 or tetrapropylammonium perruthenate (TPAP)/*N*-methylmorpholi pleased to find that diol **43** could be converted into **44** with 85 % yield under modified Swern oxidation triethylamine (TEA) or *N*,*N*-diisopropylethylamine (DIPEA) as a base).20, 21 In this case, no **46** was de

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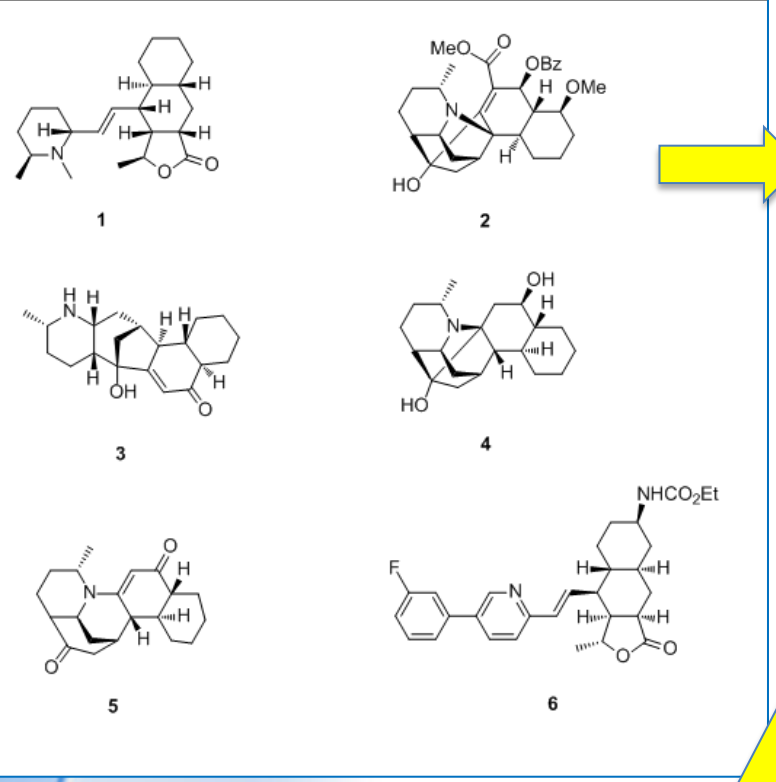
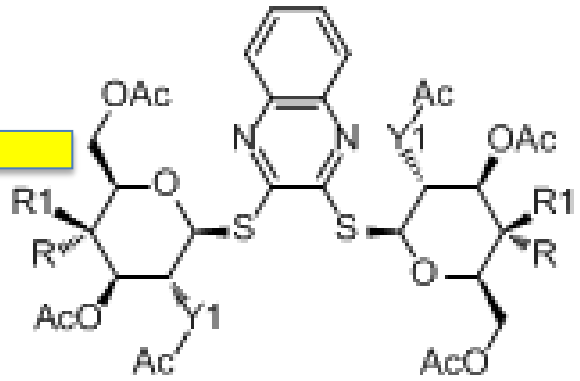
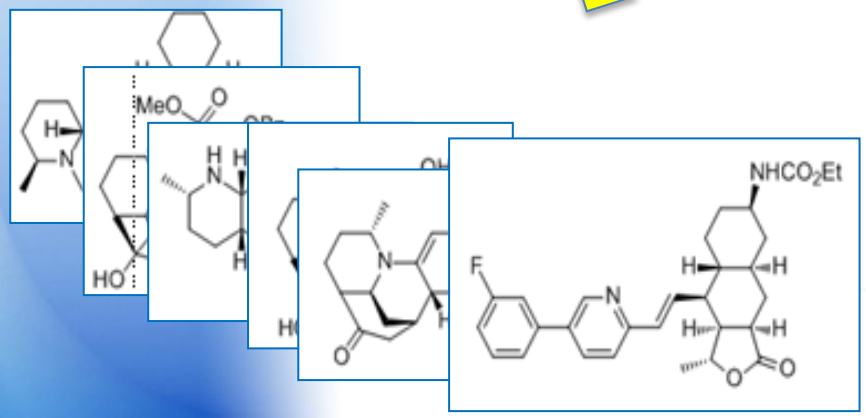


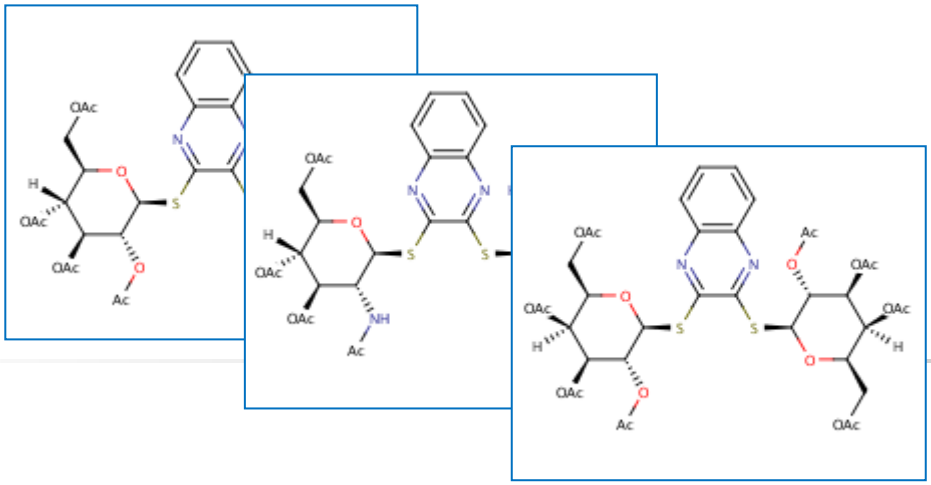
Annotation
Enumeration



Caption	R	R1	Y1
5	OAc	H	O
6	H	OAc	O
7	OAc	H	NH

SDFiles





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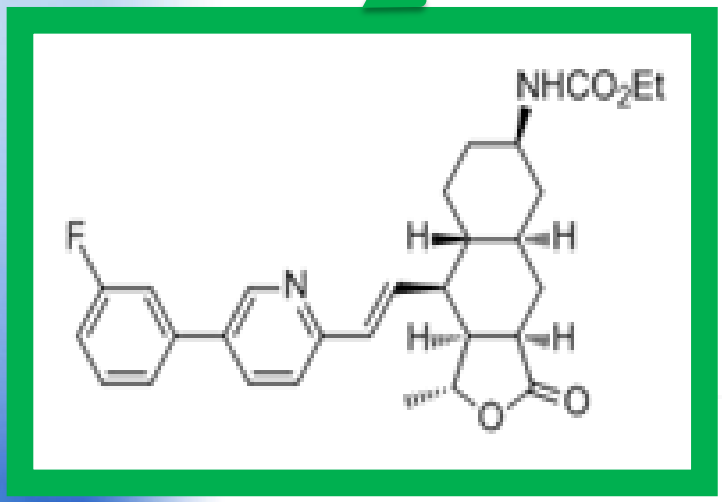

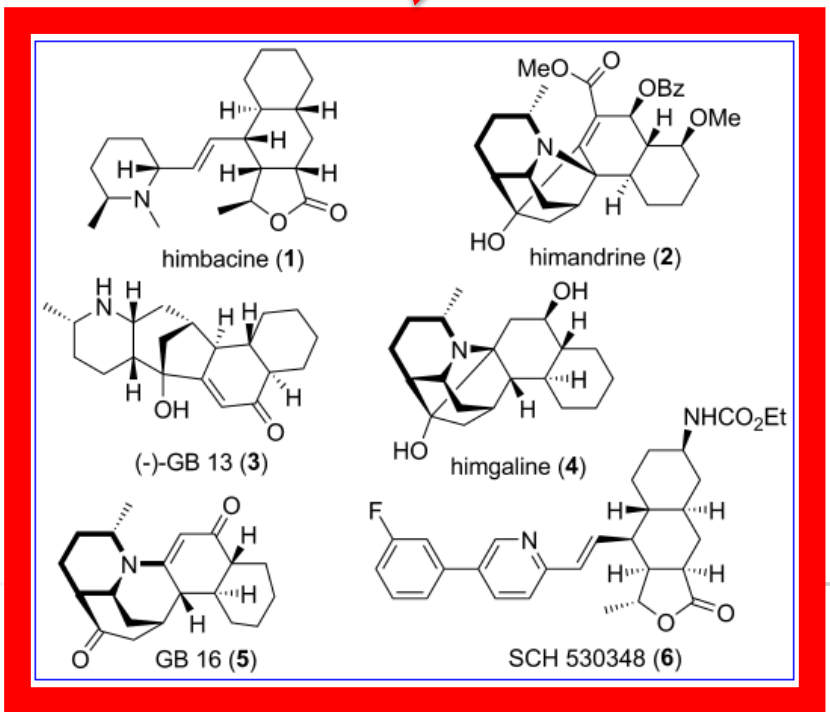

➢The Smart Article

Synthetic Studies toward **Galbulimima Alkaloid** (−)-GB 13 and (+ ...
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von W Zi - 2011 - Ähnliche Artikel
14 Dec 2010 – Himbacine (1),[1] himandrine (2),[2] **galbulimima alkaloid** 13. ((¿)-GB 13, 3),[3] and ... **galbulimima alkaloids** that were isolated from the bark of ...

Abstract | Article | References | Compound Index | Cited By

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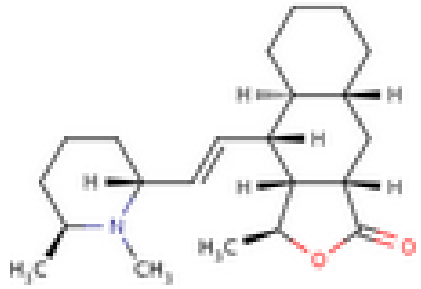
Keywords:
alkaloids; condensation; Michael addition; reductive coupling; total synthesis

Abstract

Condensation of (*S*)-3-aminobutan-1-ol with 1,3-cyclohexane-dione followed by an intramolecular alkylation afforded bicyclic enamine **32**, which was converted into enone **35** through a diastereoselective hydrogenation. Mukaiyama–Michael addition of a bicyclic silyl enol ether to **35** and subsequent stereochemistry inversion by means of an oxidation/reduction strategy provided lactone **41**. After reduction of



Compound 1

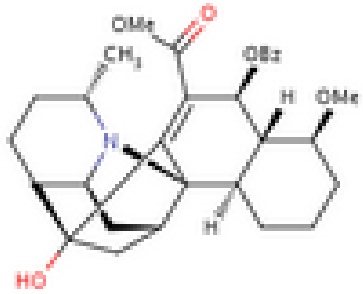
Molecular Weight: 345.5188

Molecular Formula: C22H35NO2

InChi key: FMPNFDSPHNUFOS-LPJDIUFZSA-N

View Compound

View compound in article | Full details



Compound 2

Molecular Weight: 507.6179

Molecular Formula: C30H37NO6

InChi key: YYRMLJPFAHKRJD-BJOCAQAESA-N

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Introduction

Jump to…

…e (1),1 himandrine (2),2 galbulimima alkaloid 13 ((−)-GB 13, 3),3 and himgaline (4)4 represent class I–III galbulimima alkaloids

Remove highlight
Full details

himbacine (1)

himandrine (2)

(-)-GB 13 (3)

himgaline (4)

GB 16 (5)

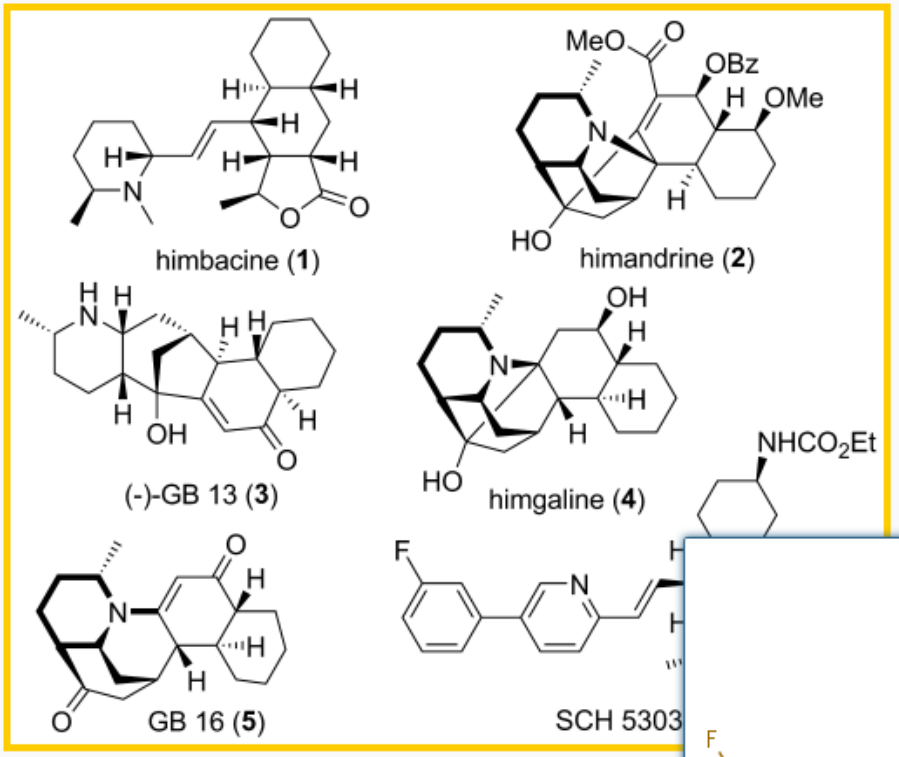
SCH 530348 (6)

that were isolated from the bark of *Galbulimima belgraveana*, a rain forest tree native to Northern Australia and Papua New Guinea. Recently, GB 16 (5),5 a new member of this family, was discovered by Mander and co-workers. These alkaloids have received great attention from the pharmaceutical industry, mainly because the *Galbulimima belgraveana* bark has been used as a medicinal substance …ine (1) has shown potent muscarinic antagonist activity.6 On the basis of a series of structure–activity relationship (SAR) …g himbacine as a leading compound, a number of thrombin receptor antagonists have been developed. Among them, SCH …is now in phase III clinic trials for treatment of acute coronary syndrome.6a

During the past decade, the fascinating structure of GB 13 has received considerable attention from synthetic chemists. This campaign has led to a number of total syntheses of himbacine,1b–d five total syntheses of GB 13,3a–e two total syntheses of himgaline,3c, d and one total synthesis of himandrine.2d For the synthesis of (±)-GB 13, Mander and McLachlan used a Diels–Alder reaction of olefin **9** and diene **10** as the key step to set up the D-ring in the intermediate **8**, and then converted the aromatic ring into the required piperidine ring

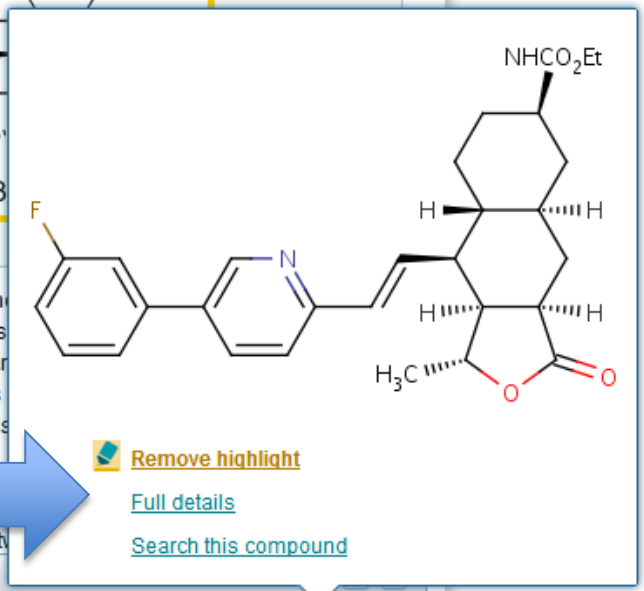
COMPOUND BROWSER 64 featured compounds in this article. (show all 82 compounds)

1 ACTIONS 2 3 4 5 6



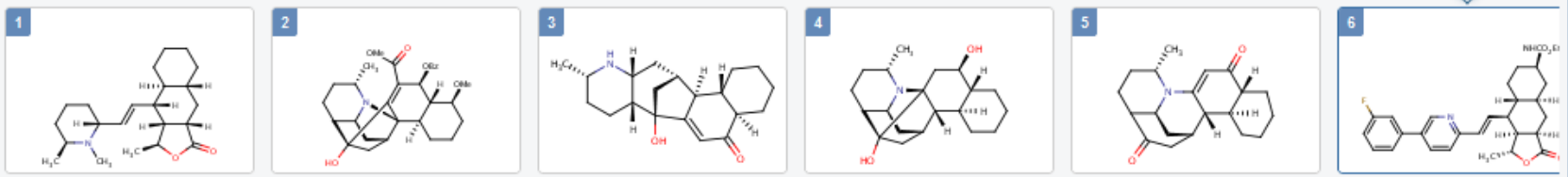
that were isolated from the bark of *Galbulimima belgraveana*, a rain forest tree native to North
Recently, GB 16 (**5**),[5] a new member of this family, was discovered by Mander and co-workers
attention from the pharmaceutical industry, mainly because the *Galbulimima belgraveana* bar
and himbacine (**1**) has shown potent muscarinic antagonist activity.[6] On the basis of a series
studies by using himbacine as a leading compound, a number of thrombin receptor antagonis
530348 (**6**) is now in phase III clinic trials for treatment of acute coronary syndrome.[6a]

During the past decade, the fasci
has led to a number of total syntheses of himbacine,[1b–d] five total syntheses of GB 13,[3a–e] t



Compound Details

COMPOUND BROWSER 64 featured compounds in this article. (show all 82 compounds)



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Wiley Smart Chemistry

Compound Record **SCH530348**

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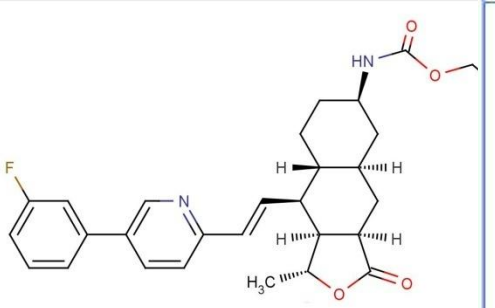

Overview | Spectra | Reactions | Chemical Tecl

Experimental Spectra:
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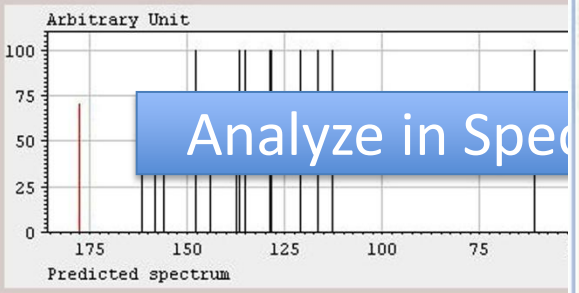
Predicted 13 CNMR Spectrum

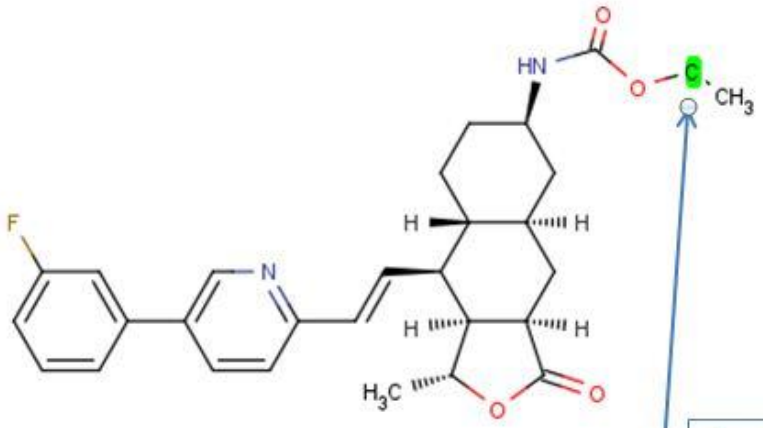


Analyze in Spec

Spectrum Prediction:

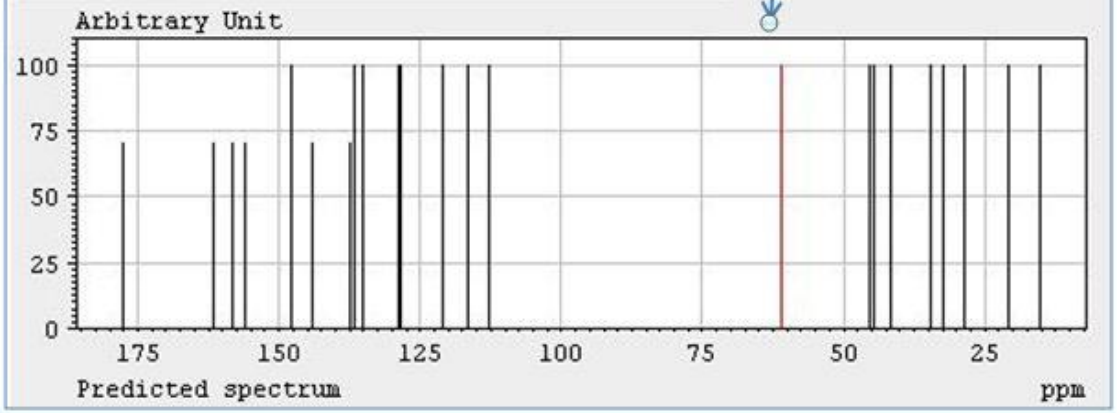
^{13}CNMR ^{1}HNMR ^{31}PNMR ^{19}FNMR ^{15}NNMR

Structure Enlarge



Assignment

^13C NMR Peak Assignment Enlarge



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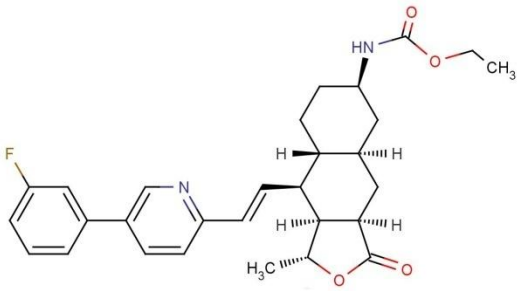
Compound Record **SCH530348**



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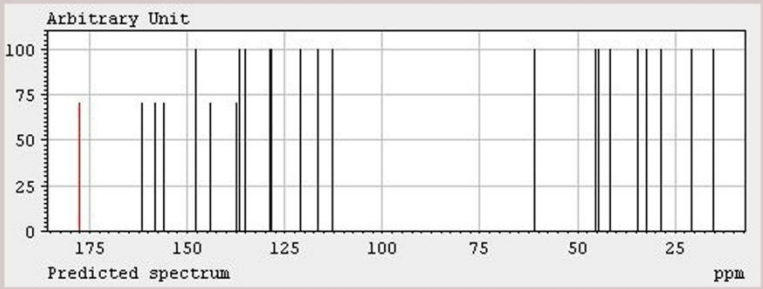
Predicted 13 CNMR Spectrum



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Spectrum Prediction:

^{13}CNMR ^{1}HNMR ^{31}PNMR ^{19}FNMR ^{15}NNMR

Other Predictions

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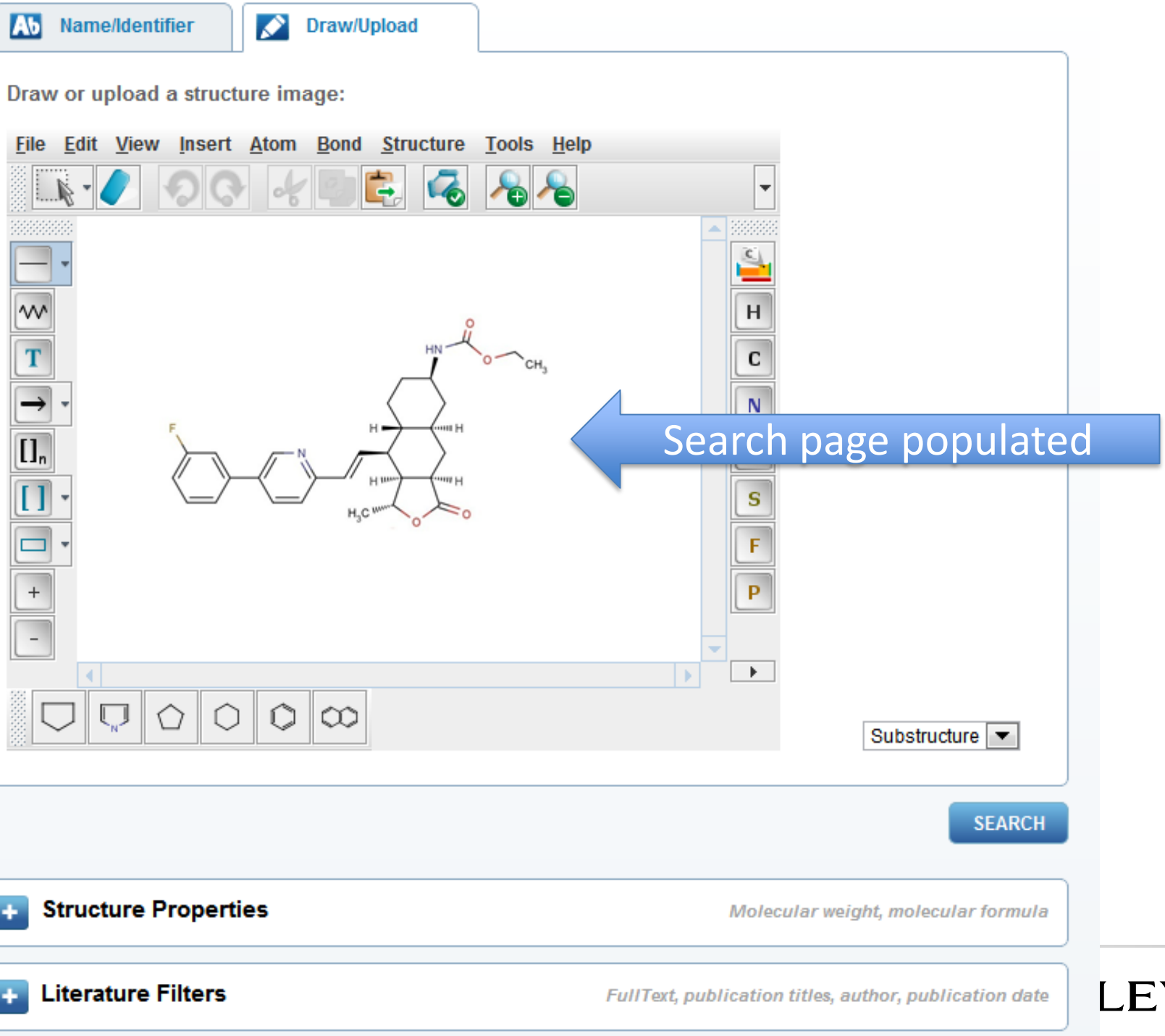
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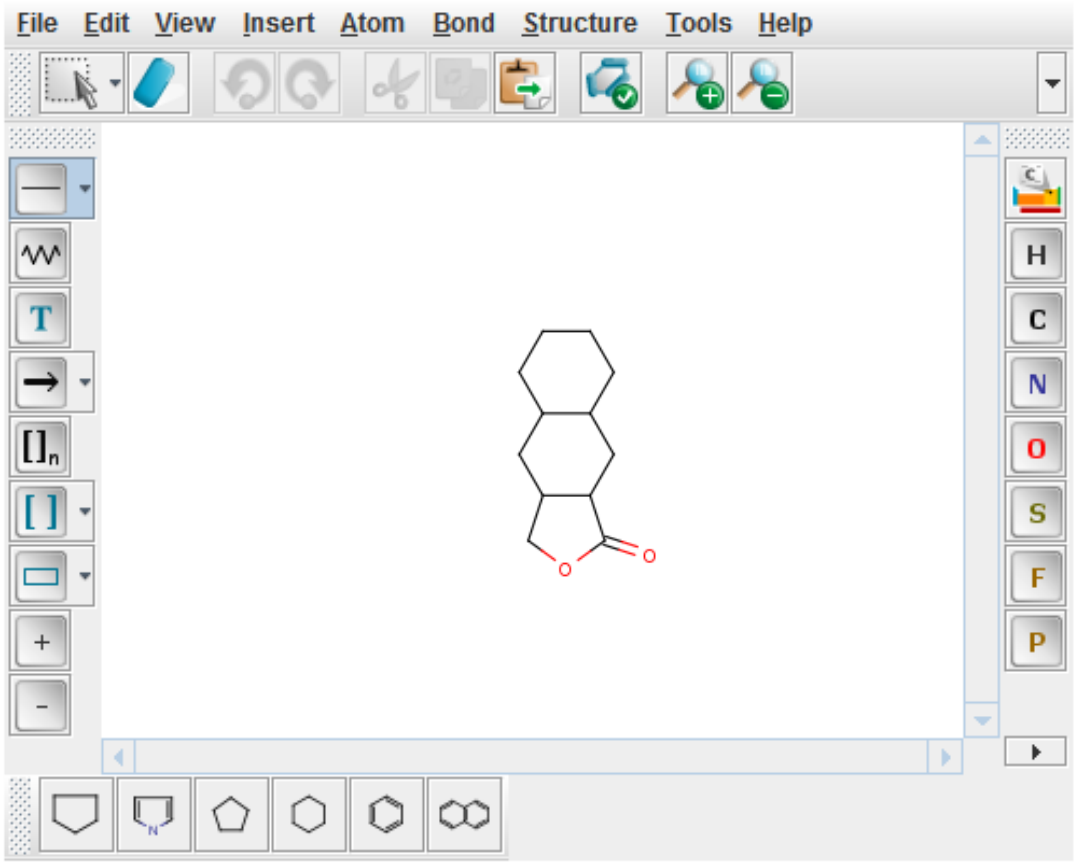

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Literature Filters *FullText, publication titles, author, publication date*

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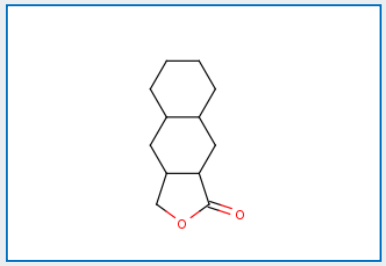

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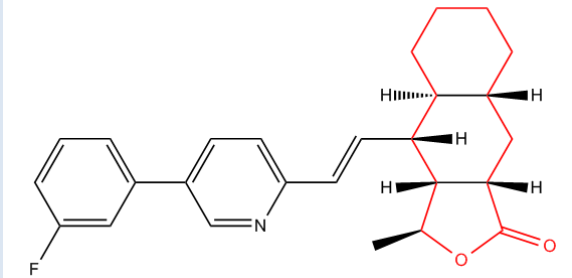
Standard Article

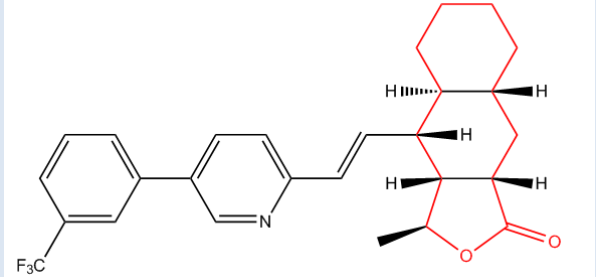
BURGER'S MEDICINAL CHEMISTRY, DRUG DISCOVERY AND DEVELOPMENT

Samuel Chackalamannil

Published Online : 15 SEP 2010, DOI: 10.1002/0471266949.bmc175

Abstract | Full Article (HTML) | PDF(2461K) | References





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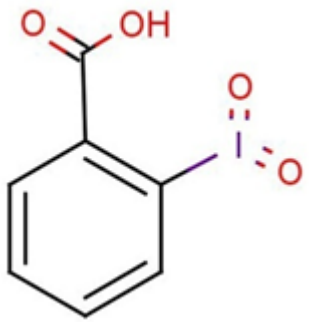

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- [x] Reagents & Catalysts
- [ ] Drug Synonyms
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diate **49**, which was oxidized with 2-iodoxybenzoic acid and then tr
.1 % over 19 linear steps. By following the known procedure, our s
starting from lactone **41**, the first total synthesis of (+)-GB 16, a nev

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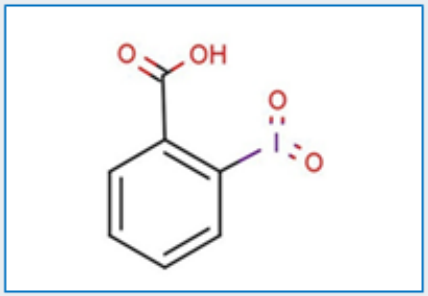

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2-Iodobenzoic Acid (IBX) Standard Article
E-EROS ENCYCLOPEDIA OF REAGENTS FOR ORGANIC SYNTHESIS
Alex G. Fallis and Pierre E. Tessier
Published Online : 15 APR 2003, DOI: 10.1002/047084289X.rn00221
Abstract Full Article (HTML) References

O-Iodobencoic acid Standard Article
FIESER AND FIESER'S REAGENTS FOR ORGANIC SYNTHESIS
Tse-Lok Ho, Mary Fieser and Louis Fieser
Published Online : 15 DEC 2006, DOI: 10.1002/9780471264194.fos05920
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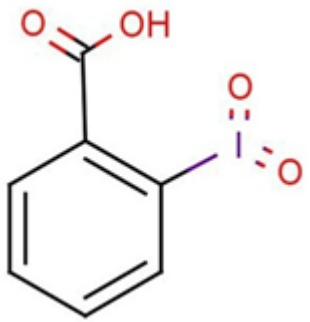

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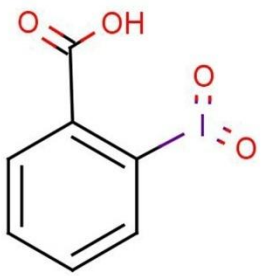

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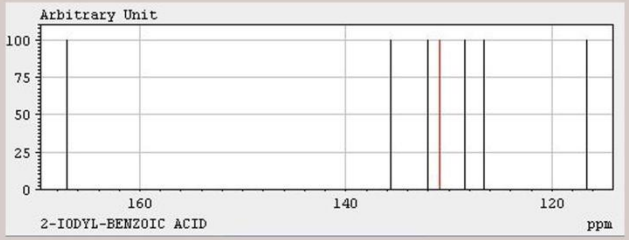

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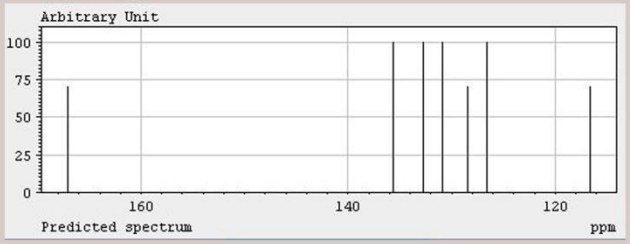
Experimental spectrum

Predicted 13 CNMR Spectrum



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Predicted spectrum

Spectrum Prediction:

^{13}CNMR ^{1}HNMR ^{31}PNMR ^{19}FNMR ^{15}NNMR

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