COMPOUND SUMMARY

Rebaudioside A

PubChem CID	6918840
Structure	 2D
Chemical Safety	Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{44}H_{70}O_{23}$
Synonyms	Rebaudioside A 58543-16-1 Stevioside A3 Rebaudioside-A Truvia View More...
Molecular Weight	967.0 g/mol *Computed by PubChem 2.1 (PubChem release 2021.05.07)*
Dates	Create: 2006-07-28 Modify: 2023-12-10
Description	Rebaudioside A is a rebaudioside that is rubusoside in which the hydroxy groups at positions 3 and 4 of the beta-D-glucopyranosyloxy group at the 13alpha position have both been converted to the corresponding beta-D-glucopyranoside. It has a role as a sweetening agent. It is a beta-D-glucoside, a tetracyclic diterpenoid and a rebaudioside. It is functionally related to a rubusoside and a beta-D-Glcp-(1->2)-[beta-D-Glcp-(1->3)]-beta-D-Glcp. ▸ ChEBI Rebaudioside A is under investigation in clinical trial NCT03510624 (Acute Effect of Rebaudioside A on Glucose Excursion During an

Oral Glucose Tolerance Test in Type 2 Diabetes Mellitus).

▸ DrugBank

Rebaudioside A is a natural product found in Stevia rebaudiana and Bos taurus with data available.

▸ LOTUS - the natural products occurrence database

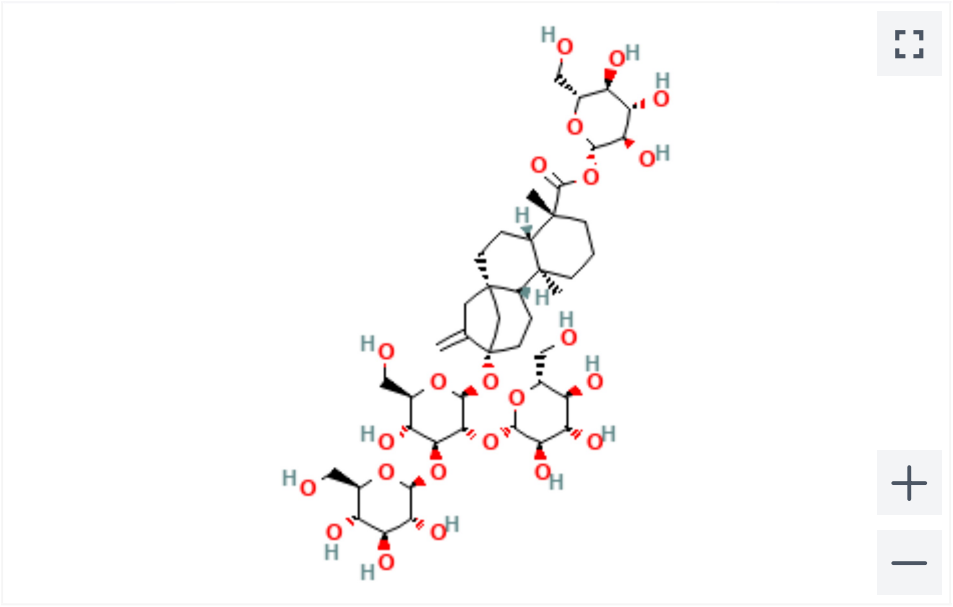
See also: Stevia rebaudiuna Leaf (part of).

1 Structures

1.1 2D Structure

Structure Search | Get Image | Download Coordinates

Chemical Structure Depiction



▸ PubChem

1.2 3D Status

Conformer generation is disallowed since too many atoms

▸ PubChem

1.3 Crystal Structures

COD records with this CID as component	4503011

- Crystallography Open Database (COD)

2 Names and Identifiers

2.1 Computed Descriptors

2.1.1 IUPAC Name

[(2*S*,3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl] (1*R*,4*S*,5*R*,9*S*,10*R*,13*S*)-13-[(2*S*,3*R*,4*S*,5*R*,6*R*)-5-hydroxy-6-(hydroxymethyl)-3,4-bis[[(2*S*,3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]oxan-2-yl]oxy-5,9-dimethyl-14-methylidenetetracyclo[11.2.1.$0^{1,10}$.$0^{4,9}$]hexadecane-5-carboxylate

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

- PubChem

2.1.2 InChI

InChI=1S/C44H70O23/c1-17-11-43-9-5-22-41(2,7-4-8-42(22,3)40(59)66-38-33(58)30(55)26(51)20(14-47)62-38)23(43)6-10-44(17,16-43)67-39-35(65-37-32(57)29(54)25(50)19(13-46)61-37)34(27(52)21(15-48)63-39)64-36-31(56)28(53)24(49)18(12-45)60-36/h18-39,45-58H,1,4-16H2,2-3H3/t18-,19-,20-,21-,22+,23+,24-,25-,26-,27-,28+,29+,30+,31-,32-,33-,34+,35-,36+,37+,38+,39+,41-,42-,43-,44+/m1/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

- PubChem

2.1.3 InChIKey

HELXLJCILKEWJH-NCGAPWICSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

- PubChem

2.1.4 Canonical SMILES

CC12CCCC(C1CCC34C2CCC(C3)(C(=C)C4)OC5C(C(C(C(O5)CO)O)OC6C(C(C(C(O6)CO)O)O)O)OC7C(C(C(C(O7)CO)O)O)O)(C)C(=O)OC8C(C(C(C(O8)CO)O)O)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.1.5 Isomeric SMILES

C[C@@]12CCC[C@@]([C@H]1CC[C@]34[C@H]2CC[C@](C3)(C(=C)C4)O[C@H]5[C@@H]([C@H]([C@@H]([C@H](O5)CO)O)O[C@H]6[C@@H]([C@H]([C@@H]([C@H](O6)CO)O)O)O)O[C@H]7[C@@H]([C@H]([C@@H]([C@H](O7)CO)O)O)O)(C)C(=O)O[C@H]8[C@@H]([C@H]([C@@H]([C@H](O8)CO)O)O)O

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

2.2 Molecular Formula

$C_{44}H_{70}O_{23}$

Computed by PubChem 2.1 (PubChem release 2021.05.07)

PubChem

2.3 Other Identifiers

2.3.1 CAS

58543-16-1

CAS Common Chemistry; ChemIDplus; DrugBank; EPA DSSTox; European Chemicals Agency (ECHA...

2.3.2 Deprecated CAS

60129-62-6, 64859-60-5, 65455-42-7

ChemIDplus

2.3.3 European Community (EC) Number

611-696-6

European Chemicals Agency (ECHA)

2.3.4 UNII

B3FUD0528F

- FDA Global Substance Registration System (GSRS)

2.3.5 DSSTox Substance ID

DTXSID8047898

- EPA DSSTox

2.3.6 FEMA Number

4601

- Flavor and Extract Manufacturers Association (FEMA)

4771

- Flavor and Extract Manufacturers Association (FEMA)

4772

- Flavor and Extract Manufacturers Association (FEMA)

2.3.7 Lipid Maps ID (LM_ID)

LMPR01040126

- LIPID MAPS

2.3.8 Metabolomics Workbench ID

143736

- Metabolomics Workbench

2.3.9 Nikkaji Number

J13.835E

- Japan Chemical Substance Dictionary (Nikkaji)

2.3.10 RXCUI

1667222