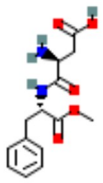
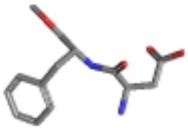
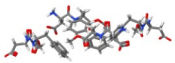
COMPOUND SUMMARY

Aspartame

PubChem CID	134601
Structure	 2D  3D  Crystal
Chemical Safety	Laboratory Chemical Safety Summary (LCSS) Datasheet
Molecular Formula	$C_{14}H_{18}N_2O_5$
Synonyms	aspartame 22839-47-0 Nutrasweet Asp-phe-ome Canderel View More...
Molecular Weight	294.30 g/mol *Computed by PubChem 2.1 (PubChem release 2021.05.07)*
Dates	Create: 2005-06-24 Modify: 2023-12-10
Description	Aspartame is a dipeptide obtained by formal condensation of the alpha-carboxy group of L-aspartic acid with the amino group of methyl L-phenylalaninate. Commonly used as an artificial sweetener. It has a role as a sweetening agent, a nutraceutical, a micronutrient, a xenobiotic, an environmental contaminant, an apoptosis inhibitor and an EC 3.1.3.1 (alkaline phosphatase) inhibitor. It is a dipeptide, a carboxylic acid and a methyl ester. It is functionally related to a L-aspartic acid and a methyl L-phenylalaninate. It is a tautomer of an aspartame zwitterion. ▸ ChEBI Flavoring agent sweeter than sugar, metabolized as phenylalanine

and aspartic acid.

▸ DrugBank

Flavoring agent sweeter than sugar, metabolized as PHENYLALANINE and ASPARTIC ACID.

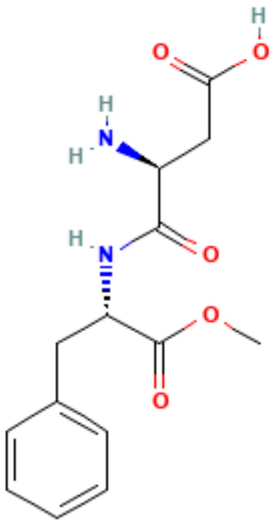
▸ Medical Subject Headings (MeSH)

1 Structures

1.1 2D Structure

Structure Search | Get Image | Download Coordinates

Chemical Structure Depiction



▸ PubChem

1.2 3D Conformer

UPDATING...

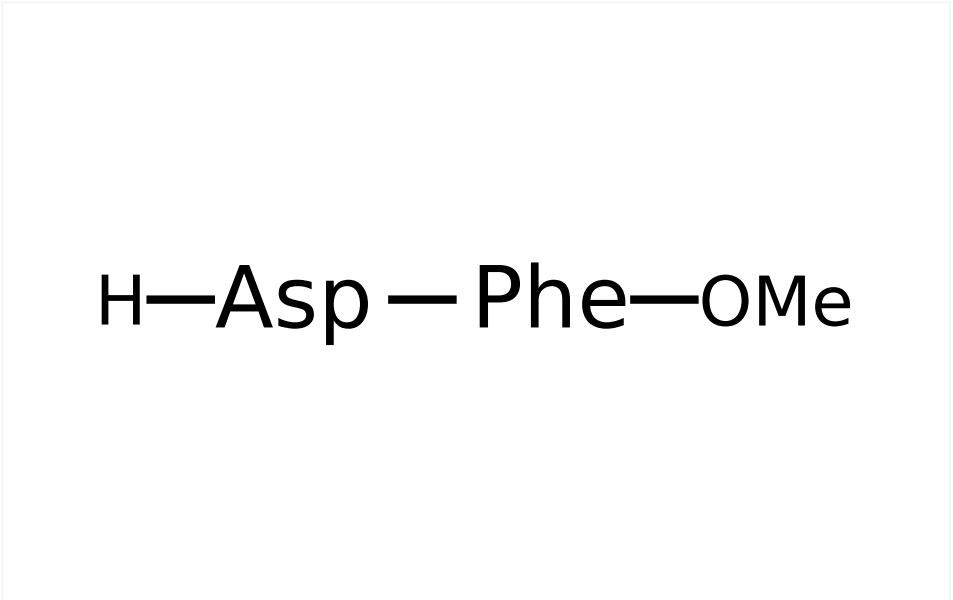
▸ PubChem

1.3 Crystal Structures

CCDC Number	608804
Associated Article	DOI:10.1021/cg060300d
Crystal Structure Data	DOI:10.5517/ccnfhvd
Crystal Structure Depiction	

▸ The Cambridge Structural Database

2 Biologic Description

SVG Image	

IUPAC Condensed	H-Asp-Phe-OMe
Sequence	DF
IUPAC	L-alpha-aspartyl-L-phenylalanine methyl ester

PubChem

3 Names and Identifiers

3.1 Computed Descriptors

3.1.1 IUPAC Name

(3*S*)-3-amino-4-[[(2*S*)-1-methoxy-1-oxo-3-phenylpropan-2-yl]amino]-4-oxobutanoic acid

Computed by Lexichem TK 2.7.0 (PubChem release 2021.05.07)

PubChem

3.1.2 InChI

InChI=1S/C14H18N2O5/c1-21-14(20)11(7-9-5-3-2-4-6-9)16-13(19)10(15)8-12(17)18/h2-6,10-11H,7-8,15H2,1H3,(H,16,19)(H,17,18)/t10-,11-/m0/s1

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.3 InChIKey

IAOZJIPTCAWIRG-QWRGUYRKSA-N

Computed by InChI 1.0.6 (PubChem release 2021.05.07)

PubChem

3.1.4 Canonical SMILES

COC(=O)C(CC1=CC=CC=C1)NC(=O)C(CC(=O)O)N

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

PubChem

3.1.5 Isomeric SMILES

COC(=O)[C@H](CC1=CC=CC=C1)NC(=O)[C@H](CC(=O)O)N

Computed by OEChem 2.3.0 (PubChem release 2021.05.07)

- PubChem

3.2 Molecular Formula

$C_{14}H_{18}N_2O_5$

Computed by PubChem 2.1 (PubChem release 2021.05.07)

- EU Food Improvement Agents; Wikipedia; PubChem

3.3 Other Identifiers

3.3.1 CAS

22839-47-0

- CAS Common Chemistry; ChemIDplus; DrugBank; DTP/NCI; EPA Chemicals under the TSCA; EPA D...

3.3.2 Deprecated CAS

53906-69-7, 7421-84-3, 172964-81-7

- ChemIDplus

7421-84-3, 53906-69-7

- EPA DSSTox

3.3.3 European Community (EC) Number

245-261-3

- EU Food Improvement Agents; European Chemicals Agency (ECHA)

3.3.4 UNII

Z0H242BBR1

- FDA Global Substance Registration System (GSRS)