



Formula: C<sub>32</sub>H<sub>44</sub>N<sub>2</sub>O<sub>8</sub>

MW: 584.71

Salt: HBr

CAS: 97792-45-5

TNP NUMBER: TNP00456

MDL NUMBER: MFCD03035011

IUPAC: (1S,3S,4S,6S,8S,9S,13S,16S)-11-ethyl-3,8-dihydroxy-4,6,16-trimethoxy-11-azahexacyclo[7.7.2.1.0.0.0]nonadec-13-yl 2-(acetylamino)benzoate

Smiles:

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c1ccc(C(O[C@@]23C4[C@]5(C6[C]7([C]([C@@H](C4)C5N(CC)C2)(C[C@@H](C([C@@H]7O)C6)OC)O)[C@H](CC3)OC)=O)c(NC(=O)C)c1
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REFERENCE: Merck 13, 5384

SOURCE: From tubers and herb of *Aconitum Seprpentroniale* Kollé, *A. orientale* mill., *A. excelsum* Reichb., *ranunculaefolium*, Ranunculaceae

ACCEPTORS: 8

DONORS: 3

ROTATION BONDS: 3

N+O: 10

Chiral Centers: 12

LogP: 2.82

LogS: -5.34

LIPINSKI: 3

Synonyms: LAPPACONITINE HBR;LAPPACONITINE  
HYDROBROMIDE;ALLAPININE;ALLAPININE  
HYDROBROMIDE;(1-alpha,14-alpha,16-beta)-monohydrobromide;allapinin;lappaconitihydrobro  
midum;LAPPACONIFINEHYDROBROIDE

CAS:97792-45-5

MF:C32H45BrN2O8

MW:665.61

EINECS:

Product Categories:Miscellaneous Natural Products LAPPACONITINE HYDROBROMIDE

Chemical Properties: mp 223-226 C storage temp. 2-8C T+ Risk Statements 28 Safety  
Statements 45 RIDADR UN 1544 6.1/PG 2 LAPPACONITINE HYDROBROMIDE

Usage And Synthesis: LAPPACONITINE HYDROBROMIDE

