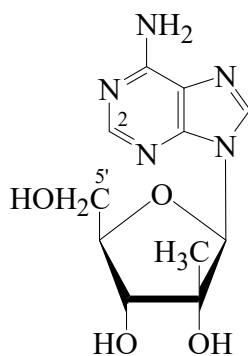




>>Entry Name: **2'-C-Methyladenosine**, 9Cl, 8Cl

Synonym(s): 9-(2-C-Methyl-β-D-ribofuranosyl)adenine



CAS Registry Number: 15397-12-3

Molecular Formula: C₁₁H₁₅N₅O₄

Molecular Weight: 281.271

Accurate Mass: 281.112405

Percentage Composition: C 46.97%; H 5.38%; N 24.90%; O 22.75%

Melting Point: Mp 257-258°

Optical Rotation: [α]_D -21 (c, 0.5 in H₂O)

Other Data: λ_{max} 260 nm (ε 15 100) (H₂O)

>>Derivative: 6*N*,2',3',5'-Tetrabenzoyl

Molecular Formula: C₃₉H₃₁N₅O₈

Molecular Weight: 697.703

Accurate Mass: 697.217265

Percentage Composition: C 67.14%; H 4.48%; N 10.04%; O 18.35%

Optical Rotation: [α]_D -66 (c, 1.0 in CHCl₃)

>>Derivative: 2',3'-*O*-Isopropylidene

Molecular Formula: C₁₄H₁₉N₅O₄

Molecular Weight: 321.335

Accurate Mass: 321.143705

Percentage Composition: C 52.33%; H 5.96%; N 21.79%; O 19.92%

Melting Point: Mp 291-292°

Optical Rotation: [α]_D -89 (c, 0.5 in MeOH)

Other Data: λ_{max} 260 nm (ε 15 100) (MeOH)

>>Derivative: 2-Chloro, 5'-deoxy

Synonym(s): 2-Chloro-5'-deoxy-2'-C-methyladenosine, 9Cl. **Kumusine**. Trachycladine A

CAS Registry Number: 164672-56-4

Molecular Formula: C₁₁H₁₄ClN₅O₃

Molecular Weight: 299.716

Accurate Mass: 299.078517

Percentage Composition: C 44.08%; H 4.71%; Cl 11.83%; N 23.37%; O 16.01%

Biological Source: Isol. from marine sponges *Theonella* sp. and *Trachycladus laevispirulifer*

Melting Point: Mp 210-213°

Optical Rotation: [α]_D -19.6 (c, 0.41 in MeOH)

UV: [neutral] λ_{max} 264 (ε 14200) (MeOH)

Other Data: Kumusine and Trachycladine A not compared. Mp refers to Kumusine, opt. rotn. to Trachycladine A

References:

Walton, E. *et al.*, *J.A.C.S.*, 1966, **88**, 4524, (*synth*)

Jenkins, S.R. *et al.*, *J.O.C.*, 1968, **33**, 2490, (*synth, pmr*)

Garrett, E.R. *et al.*, *J.A.C.S.*, 1972, **94**, 8532, (*solvolysis*)

Searle, P.A. *et al.*, *J.O.C.*, 1995, **60**, 4296-4298, (*Trachycladine A*)

Ichiba, T. *et al.*, *Tet. Lett.*, 1995, **36**, 3977-3980, (*Kumusine*)