

4228# (C15 acetogenin)

Name: (*E*)-Ocellenyne

{3-(2,3-Dibromo-pentyl)-6-pent-2-en-4-ynyl-2,5-dioxa-bicyclo[2.2.1]heptane}

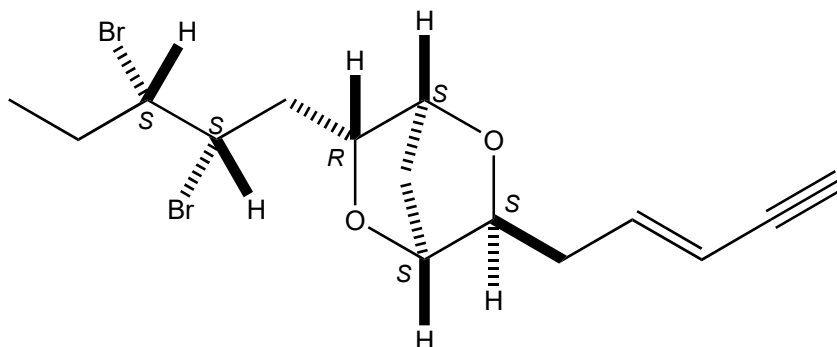
Origin: *Aplysia oculifera* (a reef flat near Pupukea, Oahu, Hawaii)⁽¹⁾;

Formula: C₁₅H₂₀Br₂O₂

Mol. Wt.: 392.13

Opt. Rot.: [α]_D²⁵ +3.21 (CHCl₃)⁽¹⁾; [α]_D²⁵ +28.5 (CHCl₃)⁽³⁾

Mp.: Colorless oil



References and Notes

(1) Schulte, G. R., Chung, M. C. H., and Scheuer, P. J. 1981. *J. Org. Chem.*, **46**, 3870-3871.

Two bicyclic C₁₅ enynes from the sea hare *Aplysia oculifera*. (UV, IR, ¹H-NMR, ¹³C-NMR, MS) (together with (*E*)-ocellenyne, (*Z*)-ocellenyne).

(2) **Revision of stereochemistry**; Jeong, D., Sohn, T., Kim, J. Y., Kim, G., Kim, D., and Paton, R. S. 2017. *Org. Lett.*, **19**, 6252-6255. Construction of 6,10-*syn*- and -*anti*-2,5-dioxabicyclo[2.2.1]heptane skeletons via oxonium ion formation/fragmentation: Prediction of structure of (*E*)-ocellenyne by NMR calculation.

(3) **Absolute configuration by total synthesis**; Hicks, H. B., Brown, D. S., Chan, H. S. S., Sousa, B. A., Christensen, K. E., and Burton, J. W. 2022. *Org. Lett.*, **24**, 9174-9178. Total synthesis and structure confirmation of (*E*) and (*Z*)-ocellenyne.