1228-1 (Sesquiterpene)

Name: Isoobtusol[1]; Iso-obtusol[4]
{2,9-Dibromo-8-chloro-1,1,9-trimethyl-5-methylene-spiro[5.5]undecan-3-ol}

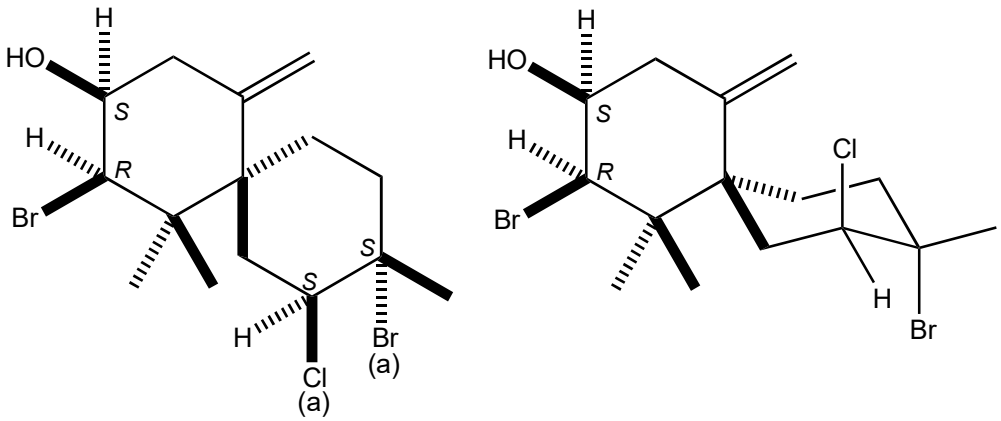
Origin: *Laurencia obtusa* (Canary Islands, Spain)[1,2,3];
Laurencia obtusa (Negril, Jamaica)[4];
Laurencia majuscula (Woodman Point, ca 30 km south of Perth, Western Australia)[4*];
Laurencia majuscula (Geoffrey Bay, Magnetic Island, Australia)[6];
Laurencia majuscula (Gran Canaria, Canary Islands, Spain)[7];
Laurencia majuscula (Pulau Satang Besar, Kuching, Sarawak, Malaysia)[8];
Laurencia majuscula (Pulau Tikus and Plau Bankawan, Sandakan, Sabah, Malaysia)[9];
Laurencia majuscula (atoll of Spratory Island, Terumbu, Layang-Layang, Malaysia)[10];
Aplysia dactylomela (the beach wrack of San Juan de la Rambla and Punta del Hidargo, Tenerife, Canary Islands, Spain)[11];

Formula: $C_{15}H_{23}Br_2ClO$

Mol. Wt.: 414.60

Opt. Rot.: $[\alpha]_D$ +33[1]; $[\alpha]_D^{26}$ +24.8 ($CHCl_3$)[7]; $[\alpha]_D^{24}$ +24.6 ($CHCl_3$)[8]

Mp.: 118-120[1]; 109-113[7]; 109-114[8]



References and Notes

(1) Gonzalez, A. G., Darias, J., Diaz, A., Fourneron, J. D., Martin, J. D., and Perez, C. 1976. Tetrahedron Lett., **17**, 3051-3054. Evidence for the biogenesis of halogenated chamigrenes from the red alga *Laurencia obtusa*. (**IR, ^{1}H-NMR**)

(2) **Structure revision**; Gonzalez, A. G., Martin, J. D., Martin, V. S., Martinez-Ripoll, M, and Fayos, J. 1979. Tetrahedron Lett., **20**, 2717-2718. X-ray study of sesquiterpene constituents of the alga *L. obtusa* leads to structure revision.

(3) Gonzalez, A. G., Martin, J. D., Martin, V. S., and Norte, M. 1979. Tetrahedron Lett., **20**, 2719-2722. Carbon-13 NMR application to *Laurencia* polyhalogenated sesquiterpenes. (**^{13}C-NMR**)

(4) Kennedy, D. J., Selby, I. A, and Thomson, R. H. 1988. Phytochemistry, **27**, 1761-1766. Chamigrane metabolites from *Laurencia obtusa* and *L. scoparia*. (**^{1}H-NMR, ^{13}C-NMR**)
(together with laurencenones A-D, deschloroelatol, elatol, iso-obtusol)

(4*) Capon, R. J., Ghisalberti, E. L., Mori, T. A., and Jefferies, P. R. 1988. J. Nat. Prod., **51**, 1302-1304. Sesquiterpenes from *Laurencia* spp. (together with obtusane, obtusol, isoobtusol, elatol)

(Continue to 1228-2)

1228-2 (Sesquiterpene) Isoobtusol

References and Notes

(Continue from 1228-1)

(5) **Stereochemistry and biogenetic consideration**; Guella, G., Oztunc, A., G, Mancini, I., and Pietra, F. 1997. Tetrahedron Lett., **38**, 8261-8264. Stereochemical features of sesquiterpene metabolites as a distinctive trait of red seaweeds in the genus *Laurencia*.

(6) de Nys, R., Coll, J. C., and Bowden, B. F. 1992. Aust. J. Chem., **45**, 1611-1623. Tropical marine algae. VIII. The structural determination of novel sesquiterpenoid metabolites from the red alga *Laurencia majuscula*. (**UV, IR, ^{1}H-NMR, ^{13}C-NMR**) (2-(3'-chloro-1',3'-dimethylcyclohexyl)-5-mehylphenol, 2-(4'-chloro-1',3'-dimethylcyclohexyl)-5-mehylphenol, 2,6,9-trimethyl-3,4,5,6-tetrahydro-2,6-methano-2*H*-1-benzoxocin-3-ol, 6 known sesquiterpenes; tricyclo[6.3.0.0^{1,5}]undecan-2-ol, isoobtusadiene, 10-bromochamigra-2,7(14)-dien-9-ol, (3(15)*E*)-10,15-dibromochamigra-1,3(15),7(14)-trien-9-ol, (3(15)*Z*)-10,15-dibromochamigra-1,3(15),7(14)-trien-9-ol, isoobtusol)

(7) Masuda, M., Kogame, K., Arisawa, S., and Suzuki, M. 1998. Botanica Marina, **40**, 265-277. Morphology and halogenated secondary metabolites of three Gran Canarian species of *Laurencia* (Ceramiales, Rhodophyta). The structures of elatol and iso-obtusol are incorrectly drawn.

(8) Vairrapan, C. S., Daitoh, M., Suzuki, M., Abe, T., and Masuda, M. 2001. Phytochemistry, **58**, 291-297. Antibacterial metabolites from the Malaysian *Laurencia* species. (**^{13}C-NMR**)

(9) Vairappan, C. S. 2003. Biomolec. Eng., **20**, 255-259. Potent antibacterial activity of halogenated metabolites from Malaysian red algae, *Laurencia majuscula* (Rhodomelaceae, Ceramiales) (together with elatol, iso-obtusol)

(10) Vairappan, C. S. and Siew-Moi, P. 2005. Malaysian J. Sci., **24**, 29-36. Morphology and halochamigrene metabolite content of *Laurencia majuscula* (Rhodomelaceae, Ceramiales) from the Spratly Islands. (together with elatol, iso-obtusol, rogiolol)

(11) **From the sea hare**; Wessels, M., Konig, G. M., and Wright, A. D. 2000. J. Nat. Prod., **63**, 920-928. New natural product isolation and comparison of the secondary metabolite content of three distinct samples of the sea hare *Aplysia dactylomela* from Tenerife. (**^{1}H-NMR, ^{13}C-NMR**)
(together with dactylopyranoid, isopinnatol B, dactylomelol, furocaespitane, puertitol B acetate, caespitenone, 8-acetylcaespitol, caespitol, caespitane, laucapyranoid A, obtusol, cartilagineol (allo-isoobtusol), 9-isoobutusol, 9-acetylisoobtusol, elatol, 9,15-dibromo-chamigra-1,3(15)-dien-11-ol)

(12) **Biological activity**; Lang, K. L., Silva, I. T., Zimmermann, L. A., Lhullier, C., Arana, M. V. M., Palermo, J. A., Falkenberg, M., Simoes, C. M. O., Schenkel, E. P., and Duran, F. J. 2012. Mar. Drugs, **10**, 2254-2264. Cytotoxic activity of semi-synthetic derivatives of elatol and isoobtusol.