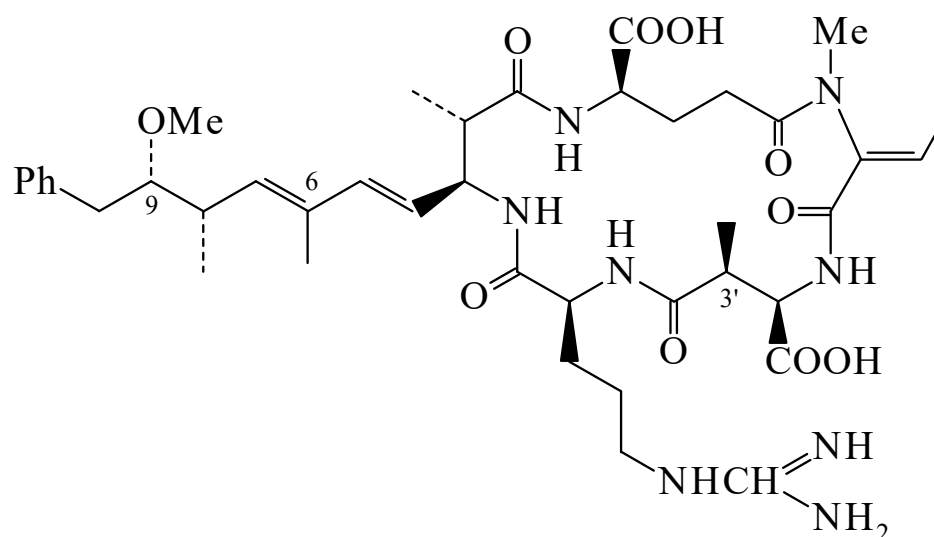




>>Entry Name: Nodularin

Synonym(s): Nodularin 1



CAS Registry Number: 118399-22-7

Molecular Formula: C<sub>41</sub>H<sub>60</sub>N<sub>8</sub>O<sub>10</sub>

Molecular Weight: 824.973

Accurate Mass: 824.443242

Percentage Composition: C 59.69%; H 7.33%; N 13.58%; O 19.39%

Biological Source: Isol. from *Nodularia spumigena*

Use/Importance: Toxin

UV: [neutral] λ<sub>max</sub> 238 (ε 33200) (MeOH) (Derep) [neutral] λ<sub>max</sub> 239 () (MeOH) (Berdy)

Other Data: Similar to Cyanoginosins

Hazard & Toxicity: BERDY HAZD : LD<sub>50</sub> (mus, ipr) .06 mg/kg

Sigma: N5148

>>Derivative: 6Z-Isomer

Synonym(s): Nodularin 3. [(6Z)-Adda<sup>3</sup>]nodularin

CAS Registry Number: 159516-66-2

Molecular Formula: C<sub>41</sub>H<sub>60</sub>N<sub>8</sub>O<sub>10</sub>

Molecular Weight: 824.973

Accurate Mass: 824.443242

Percentage Composition: C 59.69%; H 7.33%; N 13.58%; O 19.39%

Biological Source: Isol. from *Nodularia spumigena*

Optical Rotation: [α]<sub>D</sub><sup>23</sup> -63.8 (c, 0.01 in MeOH)

Hazard & Toxicity: BERDY HAZD : LD<sub>50</sub> (mus, ipr) 2 mg/kg

>>Derivative: 9-O-De-Me

Synonym(s): Nodularin 2. [DMAdda<sup>3</sup>]nodularin

CAS Registry Number: 159410-67-0

Molecular Formula: C<sub>40</sub>H<sub>58</sub>N<sub>8</sub>O<sub>10</sub>

Molecular Weight: 810.946

Accurate Mass: 810.427592

Percentage Composition: C 59.24%; H 7.21%; N 13.82%; O 19.73%

Biological Source: Isol. from *Nodularia spumigena*

Optical Rotation: [α]<sub>D</sub><sup>23</sup> -53 (c, 0.01 in MeOH)

Hazard & Toxicity: BERDY HAZD : LD<sub>50</sub> (mus, ipr) .15 mg/kg

>>Derivative: 3'-Demethyl

Synonym(s): Nodularin 4. [D-Asp<sup>1</sup>]nodularin

CAS Registry Number: 159410-68-1

Molecular Formula: C<sub>40</sub>H<sub>58</sub>N<sub>8</sub>O<sub>10</sub>

Molecular Weight: 810.946

Accurate Mass: 810.427592

Percentage Composition: C 59.24%; H 7.21%; N 13.82%; O 19.73%

Biological Source: Isol. from cultured cells (strain L-575) of *Nodularia spumigena*

Optical Rotation: [α]