



**Molecular Formula:** C<sub>18</sub>H<sub>17</sub>NO<sub>5</sub>  
**Molecular Weight:** 327.336  
**Accurate Mass:** 327.110674  
**Percentage Composition:** C 66.05%; H 5.23%; N 4.28%; O 24.44%  
**Biological Source:** Isol. from the fronds of *Athyrium filix-femina*  
**Physical Description:** Light yellow powder  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>20</sup> -20 (c, 0.7 in MeOH)

>>Derivative: *N*-Me

**CAS Registry Number:** 2566-30-5

**Molecular Formula:** C<sub>10</sub>H<sub>13</sub>NO<sub>2</sub>  
**Molecular Weight:** 179.218  
**Accurate Mass:** 179.094629  
**Percentage Composition:** C 67.02%; H 7.31%; N 7.82%; O 17.85%  
**Biological Source:** Component of Staphylomycin factor S  
**Melting Point:** Mp 260 subl.<sup>°</sup> (243-246<sup>°</sup> dec.)  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>20</sup> 0 (c, 0.5 in H<sub>2</sub>O). [ $\alpha$ ]<sub>D</sub><sup>20</sup> +21.8 (c, 0.9 in 1M HCl)  
**Sigma:** M9515

>>Derivative: *N*-Me, *N*-*tert*-butyloxycarbonyl

**CAS Registry Number:** 37553-65-4  
**Molecular Formula:** C<sub>15</sub>H<sub>21</sub>NO<sub>4</sub>  
**Molecular Weight:** 279.335  
**Accurate Mass:** 279.147059  
**Percentage Composition:** C 64.50%; H 7.58%; N 5.01%; O 22.91%  
**Physical Description:** Cryst. (EtOAc/hexane)  
**Melting Point:** Mp 85<sup>°</sup>  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>20</sup> -84.9 (c, 1 in MeOH)

>>Derivative: *N*-Me, *N*-benzyloxycarbonyl

**CAS Registry Number:** 2899-07-2  
**Molecular Formula:** C<sub>18</sub>H<sub>19</sub>NO<sub>4</sub>  
**Molecular Weight:** 313.352  
**Accurate Mass:** 313.131409  
**Percentage Composition:** C 69.00%; H 6.11%; N 4.47%; O 20.42%  
**Physical Description:** Cryst. (EtOAc/hexane)  
**Melting Point:** Mp 67-71<sup>°</sup>  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>28</sup> -67 (c, 1.8 in EtOH)

>>Derivative: *N,N*-Di-Me

**Synonym(s):** *N,N*-Dimethylphenylalanine

**CAS Registry Number:** 17469-89-5

**Molecular Formula:** C<sub>11</sub>H<sub>15</sub>NO<sub>2</sub>  
**Molecular Weight:** 193.245  
**Accurate Mass:** 193.110279  
**Percentage Composition:** C 68.37%; H 7.82%; N 7.25%; O 16.56%  
**Biological Source:** Hydrol. prod. of Canthiumine [BBW96-C](#)  
**Aldrich:** 27391-0  
**Fluka:** 41389

>>Derivative: *N,N,N*-Tri-Me, betaine

**Synonym(s):**  $\alpha$ -Carboxy-*N,N,N*-trimethylbenzeneethanaminium, 9Cl.  $\alpha$ -Trimethyl- $\beta$ -phenylpropiobetaine. Phenylalanine betaine

**CAS Registry Number:** 125982-49-2

**Molecular Formula:** C<sub>12</sub>H<sub>17</sub>NO<sub>2</sub>  
**Molecular Weight:** 207.272  
**Accurate Mass:** 207.125929  
**Percentage Composition:** C 69.54%; H 8.27%; N 6.76%; O 15.44%  
**Biological Source:** Isol. from latex and bark of *Antiaris africana*  
**Melting Point:** Mp 240-242 dec.<sup>°</sup>