

Neurosteroid Analogues. 18. Structure–activity Studies of *ent*-Steroid Potentiators of γ -Aminobutyric Acid type A Receptors and Identification of *ent*-Steroids with Activities Comparable to Those of Alphaxalone and Allopregnanolone.

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Elemental Analysis Data for Required Previously Unknown Evaluated Compounds

ent-2: Anal. (C₂₀H₃₂O₃): C, 74.96 %; H, 10.06 %. Found: C, 75.04 %; H, 9.97 %.
2: Anal. (C₂₀H₃₂O₃): C, 74.96%; H, 10.06%. Found: C, 75.04%; H, 9.93%.
ent-3: (C₂₀H₃₂O₃): C, 74.96 %; H, 10.06 %. Found: C, 75.13 %; H, 9.90 %.
3: Anal. (C₂₀H₃₂O₃): C, 74.96%; H, 10.06%. Found: C, 75.01%; H, 9.95%.
ent-7: Anal. (C₁₉H₃₀O₃): C, 78.57%; H, 10.41%; found: C, 78.36%; H, 10.58%.
7: Anal. (C₁₉H₃₀O₃): C, 78.57%; H, 10.41%; found: C, 78.78%; H, 10.61%.
ent-8: Anal. (C₂₀H₃₂O₃): C, 74.96 %; H, 10.06 %. Found: C, 74.78 %; H, 9.86 %.
8: Anal. (C₂₀H₃₂O₃): C, 74.96%; H, 10.06%; found: C, 74.69%; H, 9.91%.
ent-9: Anal. (C₂₀H₃₂O₃): C, 74.96 %; H, 10.06 %. Found: C, 75.07 %; H, 9.96%.
9: Anal. (C₂₀H₃₂O₃): C, 74.96 %; H, 10.06 %. Found: C, 75.13 %; H, 10.14%.
ent-10: Anal. (C₁₈H₂₈O₂): C, 78.21 %; H, 10.21 %. Found: C, 78.16 %; H, 10.12 %.
ent-11: Anal. (C₁₈H₂₈O₂): C, 78.21 %; H, 10.21 %. Found: C, 78.40 %; H, 10.15 %.
ent-12: Anal. (C₁₇H₂₆O₂): C, 77.82 %; H, 9.99 %. Found: C, 78.02 %; H, 9.79 %.

Optional Elemental Analysis Data for Selected Intermediate Compounds

ent-14: Anal (C₁₉H₃₀O₂): C, 78.57 %; H, 10.41 %. Found: C, 78.77%; H, 10.22%.
ent-31: Anal (C₂₉H₃₈O₄): C, 77.30 %; H, 8.50 %. Found: C, 77.55 %; H, 8.26%.
ent-32: Anal (C₂₂H₃₂O₅): C, 70.18 %; H, 8.57 %. Found: C, 70.30%; H, 8.59 %.
ent-33: Anal (C₂₀H₃₀O₃): C, 75.43 %; H, 9.50 %. Found: C, 75.17 %; H, 9.39 %.
51: Anal (C₁₉H₂₈O₄): C, 71.22 %; H, 8.81 %. Found: C, 71.12 %; H, 8.68 %.
52: Anal (C₁₇H₂₆O₂): C, 77.82 %; H, 9.99 %. Found: C, 77.69 %; H, 10.02 %
53: Anal (C₂₄H₃₂O₄S): C, 69.20 %; H, 7.74 %. Found: C, 69.09 %; H, 7.35 %.
54: Anal (C₂₅H₃₁O₃S): C, 72.42 %; H, 8.27 %. Found: C, 72.59 %; H, 8.07 %.
ent-57: Anal (C₁₇H₂₂O₂): C, 79.03 %; H, 8.58 %. Found: C, 79.09 %; H, 8.38 %.

Molecular Modeling. (A) Edge view of alignment of compounds **1** and *ent*-**1**. (B) Edge view of alignment of compounds **4** and *ent*-**1**. (C) Top view of alignment of compounds **5** and *ent*-**9**. (D) Edge view of alignment of compounds **5** and *ent*-**9**.

Figure S1

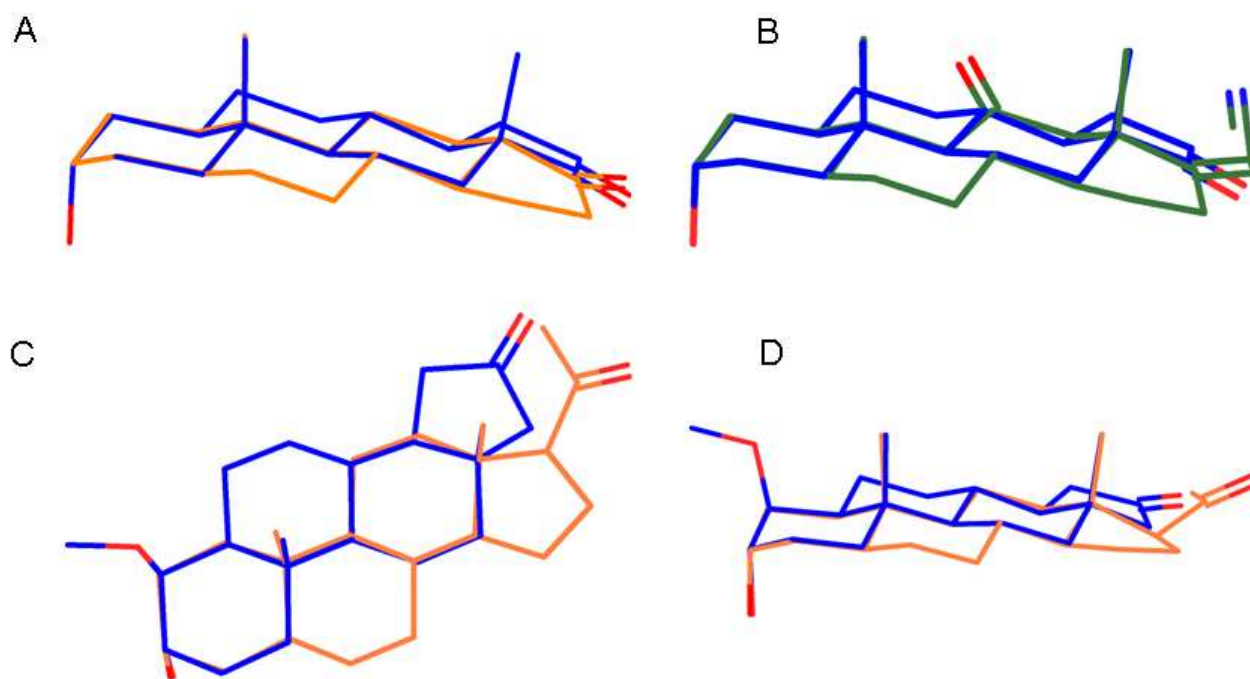


Figure S1. [³⁵S]TBPS Results. Structures of *ent*-steroids are in orientations shown for *ent*-1 in Figure 1 (i.e., α face toward the reader). Numbers in parentheses are IC₅₀ values for [³⁵S]TBPS displacement. Error limits for IC₅₀ values and slope values for binding curves are given in Table 1. Enantiomers are groups as pairs to facilitate comparison of enantiomer IC₅₀ values.

