



Supporting Information

for

Menthyl esterification allows chiral resolution for the synthesis of artificial glutamate analogs

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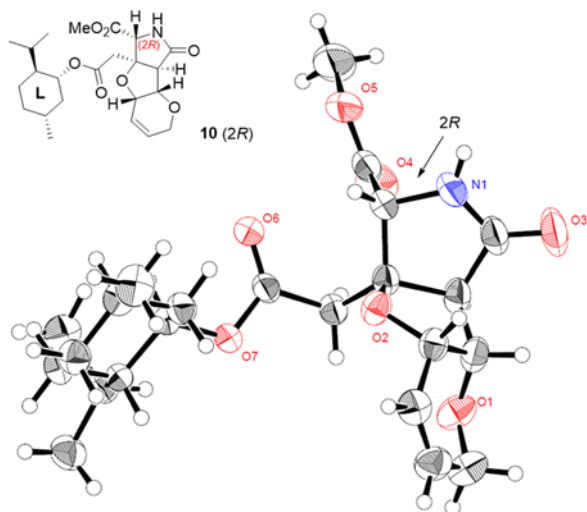
X-ray structure of the menthyl ester 10

Contents:

X-ray structure for menthyl ester 10

SIII-2 ~ SIII-6

Structure for menthyl ester 10:



CCDC accession number: 2030829

Summary for 20200831_AA70052-002

Formula: C23 H33 N1 O7

***** Unit Cell Parameters *****

a: 6.49242(16)
 b: 7.62140(18)
 c: 45.6289(11)
 alpha: 90.000
 beta: 90.000
 gamma: 90.000
 volume: 2257.78(9)

***** Model Refinement *****

R1 factor[I>2.0sigma(I)]: 0.0329
 R factor[all data]: 0.0361
 wR factor[all data]: 0.0889
 goodness of fit: 1.066
 # of observations: 4090
 # of variables: 284
 refl/para ratio: 14.4
 maximum shift/error: 0.01
 Refinement program: SHELXL 2018/3
 Refinement mode: Single
 Flack Parameter: -0.01(5)

***** Space Group Information *****

symbol: P212121
 number: 19
 centricity: acentric
 Z value: 4
 formula weight: 435.52
 calculated density: 1.281
 mu (cm⁻¹): 7.799
 crystal system: orthorhombic
 laue group: mmm
 lattice type: P

***** Reflection Corrections *****

absorption applied: Yes
 abs. type: SYM
 abs. range: 0.815-1.000
 decay applied: No
 decay (%): 0.00
 redundants averaged: Yes

***** Reflection Processing *****

total # processed: 24175
 total # unique: 4090
 R merge (%): 3.03
 Wilson B: 3.70

***** Experimental Information *****

radiation: Cu
 wavelength: 1.54187
 max. 2theta: 136.4
 sin(theta)/lambda: 0.6021
 temperature (C): -30.0

