Enantioselective Synthesis of the Anti-inflammatory Agent (−)-Acanthoic Acid

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Supporting Information

i. 1H and 13C NMR spectra for compounds:
    10, 15-18, 20, 22-25, 28-30, 32-48 and 1
    Pages 1-59

ii. X-Ray data for compounds 23, 28, 29, 41 and 42
    Pages 60-93
X-Ray data of compound 23

![Chemical structure diagram]

**Table 1. Crystal data and structure refinement for 23**

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<th>Property</th>
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<td><strong>b</strong></td>
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Table 3. Bond lengths [Å] and angles [degrees] for 23

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Table 4. Anisotropic displacement parameters [A^2 x 10^3] for 23. The anisotropic displacement factor exponent takes the form:
\[-2(\pi)^2 \left[ (ha*)^2U11 + \ldots + 2hka*b*U12 \right] \]

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S = \[ \frac{\text{GSw}(F & Vo & 0 & F & Vc & 0 & F & Vo & 0 & F & Vc & 0) & F & Vo & 0 & F & Vc & 0 & F & Vo & 0 & F & Vc & 0)}{(n - p)} \]

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X-Ray data of compound 28
Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [A^2 x 10^3] for 28. U(eq) is defined as one third of the trace of the orthogonalized U(ij) tensor.

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Table 3. Bond lengths [Å] and angles [degrees] for 28

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C(4) - C(5) 1.522 (3)  
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C(7) - C(8) 1.551 (3)  
C(7) - C(13) 1.549 (3)  
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C(8) - C(9) 1.543 (3)  
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C(11) - C(12) 1.501 (3)  
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O(1') - C(1') 1.405 (3)  
O(1') - C(3') 1.430 (3)  
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O(2') - C(3') 1.423 (3)  
O(3') - C(12') 1.219 (3)  
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O(4') - C(15') 1.446 (3)  
O(5') - C(14') 1.203 (3)  
C(1') - C(2') 1.436 (4)  
C(3') - C(4') 1.523 (3)  
C(3') - C(8') 1.559 (3)  
C(4') - C(5') 1.524 (3)  
C(5') - C(6') 1.535 (3)  
C(6') - C(7') 1.533 (3)  
C(7') - C(8') 1.550 (3)  
O(1) - C(3) 108.7 (2)  
C(3) - O(2) - C(2) 106.3 (2)  
C(14) - O(4) - C(15) 116.9 (2)  
C(1) - C(1) - C(2) 104.0 (2)  
C(2) - C(2) - C(1) 103.1 (2)  
O(2) - C(3) - O(1) 105.7 (2)  
O(2) - C(3) - C(4) 109.5 (2)  
O(1) - C(3) - C(4) 109.4 (2)  
O(2) - C(3) - C(8) 109.2 (2)  
O(1) - C(3) - C(8) 109.8 (2)  
C(4) - C(3) - C(8) 112.9 (2)  
C(5) - C(4) - C(3) 111.4 (2)  
C(4) - C(5) - C(6) 111.6 (2)  
C(5) - C(6) - C(7) 111.3 (2)  
C(6) - C(7) - C(8) 112.4 (2)  
C(6) - C(7) - C(13) 112.4 (2)  
C(8) - C(7) - C(13) 110.7 (2)  
C(10) - C(8) - C(9) 109.4 (2)  
C(10) - C(8) - C(7) 108.3 (2)  
C(9) - C(8) - C(7) 112.0 (2)  
C(10) - C(8) - C(3) 110.4 (2)  

68
C(9)–C(8)–C(3) 107.9 (2)
C(7)–C(8)–C(3) 108.9 (2)
C(11)–C(10)–C(8) 113.9 (2)
C(12)–C(11)–C(10) 113.6 (2)
O(3)–C(12)–C(11) 122.4 (2)
O(3)–C(12)–C(13) 121.3 (2)
C(11)–C(12)–C(13) 116.3 (2)
C(14)–C(13)–C(12) 108.4 (2)
C(14)–C(13)–C(7) 112.7 (2)
C(12)–C(13)–C(7) 112.0 (2)
O(5)–C(14)–O(4) 123.6 (2)
O(5)–C(14)–C(13) 124.9 (2)
O(4)–C(14)–C(13) 111.6 (2)
C(1')–O(1')–C(3') 108.6 (2)
C(2')–O(2')–C(3') 108.9 (2)
C(14')–O(4')–C(15') 116.1 (2)
O(1')–C(1')–C(2') 107.3 (2)
O(2')–C(2')–C(1') 107.8 (2)
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O(2')–C(3')–C(8') 109.1 (2)
O(1')–C(3')–C(8') 109.9 (2)
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C(6')–C(7')–C(8') 112.2 (2)
C(6')–C(7')–C(13') 112.1 (2)
C(8')–C(7')–C(13') 111.5 (2)
C(9')–C(8')–C(10') 109.4 (2)
C(9')–C(8')–C(7') 112.8 (2)
C(10')–C(8')–C(7') 108.8 (2)
C(9')–C(8')–C(3') 108.8 (2)
C(10')–C(8')–C(3') 110.3 (2)
C(7')–C(8')–C(3') 106.8 (2)
C(11')–C(10')–C(8') 113.2 (2)
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O(5')–C(14')–O(4') 124.0 (2)
O(5')–C(14')–C(13') 124.1 (2)
O(4')–C(14')–C(13') 111.9 (2)
### Table 4. Anisotropic displacement parameters [Å² x 10³]

for TAOT4&N

The anisotropic displacement factor exponent takes the form:

\[-2(\pi)^2 \left[ (ha*)^2U_{11} + \ldots + 2hka*b*U_{12} \right] \]

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-Experimental

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\[
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Table 1. Crystal data and structure refinement for 29

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<tr>
<td></td>
<td>b = 10.92(2)Å, beta = 90°</td>
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<tr>
<td></td>
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<td>Refinement method</td>
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<td>Data / restraints / parameters</td>
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<td>R indices (all data)</td>
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<td>0.274 and -0.235 e/Å³</td>
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<td>Scan speed, range, type</td>
<td>10 degrees/minute, 1.2 degrees, Wyckoff</td>
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<td>Background range, % time</td>
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X-Ray data of compound 29
Table 2. Atomic coordinates \([ x \times 10^4] \) and equivalent isotropic displacement parameters \([A^2 \times 10^3] \) for 29. \(U(eq)\) is defined as one third of the trace of the orthogonalized \(U(ij)\) tensor.

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<th>z</th>
<th>(U(eq))</th>
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Table 3. Bond lengths [Å] and angles [degrees] for 29.

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Table 4. Anisotropic displacement parameters [Å² x 10³]
for 29. The anisotropic displacement factor exponent takes the form:

\[-2(\pi)^2 [ (ha*)^2U_{11} + \ldots + 2hka*b*U_{12} ]\]

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 29.

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-Experimental
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& wR2=&GSw(F&Vo&0&^2&0-F&Vc&0&^2&0)&^2&0/&GSw[(F&Vo&0&^2&0)&^2&0]/& Gh&0,
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X-Ray data of compound 41

Table 1. Crystal data and structure refinement for 41

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Table 2. Atomic coordinates [x10^4] and equivalent isotropic displacement
parameters \([A^2 \times 10^3]\) for \(41\). U(eq) is defined as one third of the trace of the orthogonalized \(U_{ij}\) tensor.

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C(17)–C(16)–C(15)         114(2)
C(16)–C(17)–C(18)         114(2)
C(17)–C(18)–C(19)         111(2)
C(17)–C(18)–C(24)         115(2)
C(19)–C(18)–C(24)         118(2)
C(14)–C(19)–C(20)         110(2)
C(14)–C(19)–C(21)         107(2)
C(20)–C(19)–C(21)         109(2)
C(14)–C(19)–C(18)         111(2)
C(20)–C(19)–C(18)         111(2)
C(21)–C(19)–C(18)         108(2)
C(19)–C(21)–C(22)         112(2)
C(23)–C(22)–C(21)         109(2)
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C(25)–C(24)–C(26)         106(2)
C(25)–C(24)–C(23)         108(2)
C(26)–C(24)–C(23)         115(2)
C(25)–C(24)–C(18)         107(2)
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O(3)–C(26)–C(24)          126(2)
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O(1')–C(7')–C(6')         122.0(14)
O(2')–C(7')–C(6')         113.7(11)
C(7')–O(2')–C(8')         117(2)
C(26')–O(4')–C(27')       118(3)
O(2')–C(8')–C(9')         105(2)
C(11')–C(9')–C(10')       112(3)
C(11')–C(9')–C(8')        109(3)
C(10')–C(9')–C(8')        111(3)
C(11')–C(9')–C(15')       108(3)
C(10')–C(9')–C(15')       113(3)
C(8')–C(9')–C(15')        104(3)
C(12')–C(11')–C(9')       117(3)
C(11')–C(12')–C(13')      115(3)
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C(14')–C(15')–C(16')      112(3)
C(14')–C(15')–C(9')       119(3)
C(16')–C(15')–C(9')       113(3)
C(15')–C(16')–C(17')      109(3)
Table 4. Anisotropic displacement parameters [Å$^2 \times 10^3$] for 41&N. The factor exponent takes the form: $-2\pi^2[(ha^*)^2U_{11}+...+2hka^*b^*U_{12}]$

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Phenyl rings were treated as regular hexagons of D_{6h} symmetry with C-C = 1.395 Å and C-C-C = 120°. Unit cell dimensions and standard deviations were

84
obtained by least squares fit to 16 reflections (14<2 <26°).

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X-Ray data of compound 42

![Chemical structure diagram](image)

**Table 1. Crystal data and structure refinement for 42**

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<td>R indices (all data)</td>
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<td>Background range, % time</td>
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**Table 2. Atomic coordinates [x x 10⁴] and equivalent isotropic displacement parameters [Å² x 10³] for 42. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.**

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<th>U(eq)</th>
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86
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C(21)–C(19)–C(14)        111(3)
C(22)–C(21)–C(19)        112(3)
C(23)–C(22)–C(21)        111(3)
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C(23)–C(24)–C(25)        109(3)
C(23)–C(24)–C(18)        111(3)
C(25)–C(24)–C(18)        110(3)
C(23)–C(24)–C(26)        113(3)
C(25)–C(24)–C(26)        105(3)
C(18)–C(24)–C(26)        109(3)
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O(3)–C(26)–C(24)         122(4)
O(4)–C(26)–C(24)         112(3)
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C(1′)–C(2′)–C(3′)        120.0
C(4′)–C(3′)–C(2′)        120.0
C(4′)–C(3′)–Br(2)        118.7(14)
C(2′)–C(3′)–Br(2)        121.3(14)
C(3′)–C(4′)–C(5′)        120.0
C(6′)–C(5′)–C(4′)        120.0
C(5′)–C(6′)–C(1′)        120.0
C(5′)–C(6′)–C(7′)        120.1
C(1′)–C(6′)–C(7′)        119.9
O(2′)–C(7′)–O(1′)        126(2)
O(2′)–C(7′)–C(6′)        120(2)
O(1′)–C(7′)–C(6′)        113(2)
C(7′)–O(1′)–C(8′)        115(3)
C(27′)–O(4′)–C(26′)      122(3)
O(1′)–C(8′)–C(9′)        105(3)
C(8′)–C(9′)–C(11′)       111(3)
C(8′)–C(9′)–C(10′)       110(3)
C(11′)–C(9′)–C(10′)      109(3)
C(10′)–C(9′)–C(15′)      108(3)
C(11′)–C(9′)–C(15′)      109(3)
C(12′)–C(11′)–C(9′)      114(3)
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C(15′)–C(14′)–C(19′)     115(4)
C(14′)–C(15′)–C(16′)     111(3)
C(14′)–C(15′)–C(9′)      113(3)
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C(17′)–C(16′)–C(15′)     106(3)
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C(17′)–C(18′)–C(24′)     113(3)
C(14′)–C(19′)–C(18′)     109(3)
C(14′)–C(19′)–C(21′)     115(3)
C(18′)–C(19′)–C(21′)     108(3)
C(14′)–C(19′)–C(20′)     107(3)
Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters \([\text{Å}^2 \times 10^3]\) for 42. The factor exponent takes the form: 

\[-2\pi^2 \left( h^2 U_{11} + \ldots + 2hka*b*U_{12} \right)\]

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Table 5. Hydrogen coordinates \((x \times 10^4)\) and isotropic displacement parameters \((\text{Å}^2 \times 10^3)\) for 42.

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Phenyl rings were treated as regular hexagons of D$_{6h}$ symmetry with C-C = 1.395 Å and C-C-C = 120°. Unit cell dimensions and standard deviations were obtained by least squares fit to 14 reflections (14<2θ<22°).
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