Supporting Information File 2

Title: CIF data of arjuna-bromolactone 3

A simple route for renewable nano-sized arjunolic and asiatic acids and self-assembly of arjuna-bromolactone

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D 44780 Bochum, Germany
E-mail: william.sheldrick@ruhr-uni-bochum.de

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Version 1.171.32.4 (release 27-04-2006 CrysAlis171 .NET)
(compiled Apr 27 2007,17:53:11)
Empirical absorption correction using spherical harmonics,
implemented in SCALE3 ABSPACK scaling algorithm.
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F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2^ are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
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C03 C 0.62649(15) 0.84509(14) 0.54516(10) 0.0147(4) Uani 1 1 d . . .
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C09 C 0.42507(15) 0.90296(13) 0.91490(11) 0.0109(4) Uani 1 1 d . . .
C10 C 0.31434(14) 0.92384(14) 0.95441(11) 0.0134(4) Uani 1 1 d . . .
H10A H 0.2943 0.9929 0.9428 0.016 Uiso 1 1 calc R . .
H10B H 0.2603 0.8810 0.9279 0.016 Uiso 1 1 calc R . .
C11 C 0.31058(14) 0.90701(14) 1.04836(11) 0.0148(4) Uani 1 1 d . . .
H11A H 0.3131 0.8355 1.0596 0.018 Uiso 1 1 calc R . .
H11B H 0.2419 0.9325 1.0701 0.018 Uiso 1 1 calc R . .
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C13 C 0.51000(15) 0.91186(13) 1.06600(11) 0.0125(4) Uani 1 1 d . . .
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C14 C 0.51169(15) 0.94716(13) 0.97396(11) 0.0109(4) Uani 1 1 d . . .
C15 C 0.62317(14) 0.96205(13) 0.93855(11) 0.0146(4) Uani 1 1 d . . .
H15 H 0.6596 1.0126 0.9734 0.018 Uiso 1 1 calc R . .
C16 C 0.62494(15) 0.99937(14) 0.85062(10) 0.0138(4) Uani 1 1 d . . .
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H16B H 0.6022 1.0691 0.8498 0.017 Uiso 1 1 calc R . .
C17 C 0.55088(14) 0.93925(13) 0.79460(10) 0.0109(4) Uani 1 1 d . . .
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C18 C 0.57498(14) 0.95554(13) 0.70065(10) 0.0112(4) Uani 1 1 d . . .
C19 C 0.50210(17) 0.98615(14) 0.50677(11) 0.0187(4) Uani 1 1 d . . .
H19A H 0.5649 1.0277 0.5165 0.028 Uiso 1 1 calc R . .
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C20 C 0.39463(16) 1.05879(14) 0.82140(11) 0.0152(4) Uani 1 1 d . . .
H20A H 0.3975 1.0828 0.7645 0.023 Uiso 1 1 calc R . .
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H21A H 0.4633 0.7654 0.9633 0.026 Uiso 1 1 calc R . .
H21B H 0.4928 0.7747 0.8676 0.026 Uiso 1 1 calc R . .
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C22 C 0.57790(16) 1.06626(14) 0.67793(11) 0.0166(4) Uani 1 1 d . . .
H22A H 0.6266 1.0763 0.6314 0.025 Uiso 1 1 calc R . .
H22B H 0.6030 1.1043 0.7254 0.025 Uiso 1 1 calc R . .
H22C H 0.5059 1.0881 0.6626 0.025 Uiso 1 1 calc R . .
C23 C 0.43209(16) 0.81984(14) 0.51482(11) 0.0177(4) Uani 1 1 d . . .
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H23B H 0.4563 0.8053 0.4580 0.021 Uiso 1 1 calc R . .

C24 C 0.41520(14) 1.05854(14) 1.05725(11) 0.0134(4) Uani 1 1 d . . .
C25 C 0.39289(16) 0.95650(15) 1.18781(11) 0.0174(4) Uani 1 1 d . . .
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H25B H 0.4469 1.0009 1.2125 0.021 Uiso 1 1 calc R . .
C26 C 0.40851(17) 0.85254(16) 1.22133(11) 0.0212(4) Uani 1 1 d . . .
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H26B H 0.4070 0.8550 1.2823 0.025 Uiso 1 1 calc R . .
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C28 C 0.52126(17) 0.80637(14) 1.09821(12) 0.0181(4) Uani 1 1 d . . .
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are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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