SUPPLEMENTARY MATERIAL

Isolation, structural elucidation and cytotoxicity evaluation of a new pentahydroxy-pimarane diterpenoid along with other chemical constituents from *Aerva lanata*

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Abstract: *Aerva lanata* possesses various useful medicinal and pharmaceutical activities. Phytochemical investigation of the plant has now led to the isolation of a new 2 α ,3 α ,15,16,19-pentahydroxy pimar-8(14)-ene diterpenoid (**1**) together with 12 other known compounds identified as β -sitosterol (**2**), β -sitosterol-3-*O*- β -D-glucoside (**3**), canthin-6-one (**4**), 10-hydroxycanthin-6-one (aervine, **5**), 10-methoxycanthin-6-one (methylaervine, **6**), β -carboline-1-propionic acid (**7**), 1-*O*- β -D-glucopyranosyl-(2*S*,3*R*,8*E*)-2-[(2'*R*)-2'-hydroxypalmitoylamino]-8-octadecene-1, 3-diol (**8**), 1-*O*-(β -D-glucopyranosyl)-(2*S*,3*S*,4*R*,8*Z*)-2-[(2'*R*)-2'-hydroxytetracosanoylamino]-8(*Z*)-octadene-1,3,4-triol (**9**), (2*S*,3*S*,4*R*,10*E*)-2-[(2'*R*)-2'-hydroxytetracosanoylamino]-10-octadecene-1,3,4-triol (**10**), 6'-*O*-(4''-hydroxy-trans-cinnamoyl)-kaempferol-3-*O*- β -D-glucopyranoside (tribuloside, **11**), 3-cinnamoyltribuloside (**12**) and sulfonoquinovosyldiacylglyceride (**13**). Among these, six compounds (**8-13**) are reported for the first time from this plant. Cytotoxicity evaluation of the compounds against five cancer cell lines (CHO, HepG2, HeLa, A-431 and MCF-7) shows promising IC₅₀ values for compounds **4**, **6** and **12**.

Keywords: *Aerva lanata*; Pimarane diterpenoid; 2D-NMR (HSQC, HMBC, COSY, NOESY); Cytotoxicity

Experimental Section

Cytotoxicity assay:

Cell lines (CHO, HepG2, HeLa, A-431 and MCF-7) were obtained from National Centre for Cell Sciences, Pune, India. MEM-alpha, FBS (foetal bovine serum), penicillin – streptomycin were purchased from Gibco, India. Cell culture flasks, plates, tips were obtained from Tarsons, Kolkata, India. DMEM, other components of media and all other chemicals were purchased from Sigma, St Louis, USA.

Cell lines were maintained in DMEM media containing 10% FBS and 40µg/ml gentamycin. HeLa cells were plated (in 96 well plates) at 6000 cells/well/180µl media. For other cell lines it was 4000 cells/well/180µl media. Cell seeding density was optimized so that the wells without any inhibitor can make up to 90% confluency at the end of incubation period / experiment. The plates containing cells were placed in 37°C incubator with 5% CO₂ and 95% relative humidity for 24h. Media was aspirated off and replaced with 180µl fresh media. Test compounds were dissolved at conc. of 5mM (in DMSO) and further serial half dilutions were made in DMSO to reach to conc. of 0.078mM. These sub-stocks were further 10 fold diluted in respective growth media. Then 20µl of growth media containing test compounds was added (n=2) in 96-well test plate to produce final working conc. of 50 to 0.78µM (DMSO: 1%). Each plate had cell control, vehicle control, media control and standard inhibitor Doxorubicin at 10µM.

The plates were put back to incubator for 72hrs. A 20µl aliquot of MTT (5mg/ml of PBS pH7.2) was added in each well and the plates were further incubated for 4hrs. These were centrifuged (2500rpm, 10min), media flicked off and formazan crystals dissolved in 150µl DMSO. Absorbance was measured at 510nm using Spectramax M5 (Molecular Devices, USA). Cell death at each conc was determined based on OD difference of the test well from that of wells of vehicle control. If the highest test conc (50µM) showed less than 50% cell death then IC₅₀ (concentration that causes 50% cell death) is reported as > 50µM or else it was calculated using GraphPad Prism 5.0 software. The MTT assay experiment was performed in duplicate wells each day and on three separate days (Talupula [2011](#); Al-Qubaisi et al. [2011](#)).

Figure S1. Selected ^1H - ^1H COSY (—) and HMBC (H $\rightarrow$ C) correlations of compound **1**

Figure S2. Selected NOESY correlations of compound **1**

Figure S3. X-ray crystal packing cell of compound **1**

Table S1. ^1H , ^{13}C NMR and selected correlation spectral data of **1***.

Carbon No	δ_{C} (CHn)	HSQC ($^{13}\text{C} \times ^1\text{H}$)	HMBC (C $\rightarrow$ H)	HMBC (H $\rightarrow$ C)	COSY ($^1\text{H} \times ^1\text{H}$)	NOESY ($^1\text{H} \times ^1\text{H}$)
1	41.7	2.16, 2.02	H-3, H-20	C-2, C-10, C-20	H-20	H-20
2	66.9	4.51	H-3, H-1		H-3	H-3, H-20, H-19
3	74.4	4.68	H-19, H-18, H-5	C-2, C-1, C-5, C-18, C-19	H-2	H-2, H-19
4	45.5	-	H-19, H-3, H-18	-	-	-
5	49.3	1.99	H-3, H-20, H-7, H-9	C-3, C-6, C-7, C-10, C-20	H-6	H-9, H-6, H-18
6	22.7	1.73, 1.46	H-5, H-7	C-5, C-7, C-8, C-10	H-5, H-7	H-18, H-5
7	36.9	2.33, 2.12	H-14, H-5	C-6, C-8, C-9, C-14	H-6, H-14	H-14, H-5, H-9
8	137.7	-	H-7, H-9, H-6, H-14	-	-	-
9	51.6	1.96	H-14, H-7, H-20	C-5, C-8, C-11, C-20	H-11, H-14	H-5, H-11
10	39.5	-	H-5, H-20, H-1, H-9	-	-	-
11	19.5	1.71, 1.58	H-12, H-9	C-9, C-8, C-12, C-13	H-9, H-12	H-9, H-20, H-17
12	31.3	1.78, 1.54	H-14, H-15, H-17	C-11, C-13, C-17	H-11	H-11, H-17
13	38.8	-	H-14, H-15, H-17	-	-	-
14	129.6	5.71	H-15, H-7, H-17	C-7, C-8, C-12, C-13, C-15	H-7, H-9	H-16, H-7
15	80.1	3.87	H-14, H-16, H-17	C-12, C-13, C-14, C-16, C-17	H-16	H-16
16	63.8	4.19, 3.95	H-15	C-15, C-13	H-15	H-15, H-14
17	23.5	1.23	H-14, H-15, H-12	C-12, C-13, C-14, C-15	H-11	H-11, H-12
18	24.1	1.65	H-3, H-19, H-5	C-3, C-4, C-19	-	H-5, H-6
19	65.4	4.21, 3.85	H-3, H-5, H-18	C-3, C-4, C-18	-	H-2, H-3
20	17.3	0.97	H-1, H-5, H-9	C-1, C-5, C-9, C-10	H-1	H-1, H-2, H-11

* Assignments based on ^{13}C , DEPT, HSQC, HMBC, COSY, NOESY experiments

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150.47

136.13

129.60

124.09

80.14

74.42

66.90

51.65

49.26

160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

4Soc

HMBC

NOESY

Comment: Sample in KBr

Bruker FTIR, TENSOR 27

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C20 0.047(3) 0.031(2) 0.043(3) -0.0013(19) -0.001(2) -0.0002(19)
C15 0.048(3) 0.044(2) 0.033(3) 0.001(2) 0.008(2) 0.000(2)
C12 0.035(3) 0.061(3) 0.037(3) -0.002(2) 0.007(2) -0.005(3)
C17 0.055(4) 0.044(3) 0.058(4) -0.004(3) 0.006(3) -0.002(3)
O5 0.052(3) 0.093(3) 0.058(3) 0.036(3) 0.001(2) -0.008(2)
O7 0.053(3) 0.068(2) 0.042(2) 0.0022(19) 0.0039(18) 0.017(2)
O6 0.066(3) 0.058(2) 0.046(2) 0.0028(19) 0.001(2) -0.001(2)

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All esds (except the esd in the dihedral angle between two l.s. planes) 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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C3 O2 1.430(6) . ?
C3 C2 1.523(7) . ?
C3 C4 1.526(7) . ?
C3 H3 0.9800 . ?
O3 C19 1.435(7) . ?
O3 H3A 0.8200 . ?
O1 C2 1.447(6) . ?
O1 H1 0.8200 . ?
O2 H2 0.8200 . ?
C5 C10 1.544(7) . ?
C5 C6 1.545(6) . ?
C5 C4 1.566(7) . ?
C5 H5 0.9800 . ?
C1 C2 1.515(7) . ?
C1 C10 1.548(6) . ?
C1 H1A 0.9700 . ?
C1 H1B 0.9700 . ?
C10 C20 1.541(6) . ?
C10 C9 1.567(6) . ?
C4 C18 1.515(7) . ?
C4 C19 1.536(7) . ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C2 H2A 0.9800 . ?
C19 H19A 0.9700 . ?
C19 H19B 0.9700 . ?
C8 C14 1.337(7) . ?
C8 C7 1.510(8) . ?
C8 C9 1.514(7) . ?
C9 C11 1.517(7) . ?
C9 H9 0.9800 . ?
C13 C14 1.514(8) . ?
C13 C12 1.530(7) . ?
C13 C17 1.534(7) . ?
C13 C15 1.552(7) . ?
C16 O5 1.410(7) . ?
C16 C15 1.510(7) . ?
C16 H16A 0.9700 . ?
C16 H16B 0.9700 . ?
C14 H14 0.9300 . ?
O4 C15 1.458(7) . ?

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O4 H4 0.8200 . ?
 C11 C12 1.512(7) . ?
 C11 H11A 0.9700 . ?
 C11 H11B 0.9700 . ?
 C6 C7 1.523(7) . ?
 C6 H6A 0.9700 . ?
 C6 H6B 0.9700 . ?
 C7 H7A 0.9700 . ?
 C7 H7B 0.9700 . ?
 C20 H20A 0.9600 . ?
 C20 H20B 0.9600 . ?
 C20 H20C 0.9600 . ?
 C15 H15 0.9800 . ?
 C12 H12A 0.9700 . ?
 C12 H12B 0.9700 . ?
 C17 H17A 0.9600 . ?
 C17 H17B 0.9600 . ?
 C17 H17C 0.9600 . ?
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 O2 C3 C4 112.0(4) . . ?
 C2 C3 C4 111.5(4) . . ?
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 C2 C3 H3 109.1 . . ?
 C4 C3 H3 109.1 . . ?
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 C2 O1 H1 109.5 . . ?
 C3 O2 H2 109.5 . . ?
 C10 C5 C6 110.7(4) . . ?
 C10 C5 C4 117.3(4) . . ?
 C6 C5 C4 113.2(4) . . ?
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 C4 C5 H5 104.8 . . ?
 C2 C1 C10 112.1(4) . . ?
 C2 C1 H1A 109.2 . . ?
 C10 C1 H1A 109.2 . . ?
 C2 C1 H1B 109.2 . . ?
 C10 C1 H1B 109.2 . . ?
 H1A C1 H1B 107.9 . . ?
 C20 C10 C5 113.7(4) . . ?
 C20 C10 C1 109.9(4) . . ?
 C5 C10 C1 108.8(4) . . ?
 C20 C10 C9 109.0(4) . . ?
 C5 C10 C9 107.4(4) . . ?
 C1 C10 C9 107.9(4) . . ?
 C18 C4 C3 108.5(4) . . ?
 C18 C4 C19 108.2(4) . . ?
 C3 C4 C19 109.7(4) . . ?

C18 C4 C5 109.1(4) . . ?
 C3 C4 C5 108.9(4) . . ?
 C19 C4 C5 112.4(4) . . ?
 C4 C18 H18A 109.5 . . ?
 C4 C18 H18B 109.5 . . ?
 H18A C18 H18B 109.5 . . ?
 C4 C18 H18C 109.5 . . ?
 H18A C18 H18C 109.5 . . ?
 H18B C18 H18C 109.5 . . ?
 O1 C2 C1 110.4(4) . . ?
 O1 C2 C3 107.9(4) . . ?
 C1 C2 C3 111.3(4) . . ?
 O1 C2 H2A 109.1 . . ?
 C1 C2 H2A 109.1 . . ?
 C3 C2 H2A 109.1 . . ?
 O3 C19 C4 112.4(4) . . ?
 O3 C19 H19A 109.1 . . ?
 C4 C19 H19A 109.1 . . ?
 O3 C19 H19B 109.1 . . ?
 C4 C19 H19B 109.1 . . ?
 H19A C19 H19B 107.9 . . ?
 C14 C8 C7 121.1(5) . . ?
 C14 C8 C9 123.1(5) . . ?
 C7 C8 C9 115.8(4) . . ?
 C8 C9 C11 111.1(4) . . ?
 C8 C9 C10 111.3(4) . . ?
 C11 C9 C10 114.1(4) . . ?
 C8 C9 H9 106.6 . . ?
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 C14 C13 C12 108.3(4) . . ?
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 C12 C13 C15 108.9(4) . . ?
 C17 C13 C15 111.5(4) . . ?
 O5 C16 C15 109.1(5) . . ?
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 C15 C16 H16A 109.9 . . ?
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 H16A C16 H16B 108.3 . . ?
 C8 C14 C13 125.6(5) . . ?
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 C5 C6 H6B 109.8 . . ?
 H6A C6 H6B 108.2 . . ?

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C8 C7 C6 113.8(4) . . ?
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C6 C7 H7A 108.8 . . ?
C8 C7 H7B 108.8 . . ?
C6 C7 H7B 108.8 . . ?
H7A C7 H7B 107.7 . . ?
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C10 C20 H20B 109.5 . . ?
H20A C20 H20B 109.5 . . ?
C10 C20 H20C 109.5 . . ?
H20A C20 H20C 109.5 . . ?
H20B C20 H20C 109.5 . . ?
O4 C15 C16 110.0(4) . . ?
O4 C15 C13 110.7(4) . . ?
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O4 C15 H15 106.5 . . ?
C16 C15 H15 106.5 . . ?
C13 C15 H15 106.5 . . ?
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H12A C12 H12B 107.8 . . ?
C13 C17 H17A 109.5 . . ?
C13 C17 H17B 109.5 . . ?
H17A C17 H17B 109.5 . . ?
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C10 C5 C4 C19 -72.3(5) . . . . ?
C6 C5 C4 C19 58.5(6) . . . . ?
C10 C1 C2 O1 -179.7(4) . . . . ?
C10 C1 C2 C3 -59.9(5) . . . . ?
O2 C3 C2 O1 59.9(5) . . . . ?
C4 C3 C2 O1 -178.0(4) . . . . ?
O2 C3 C2 C1 -61.3(5) . . . . ?
C4 C3 C2 C1 60.8(5) . . . . ?
C18 C4 C19 O3 -47.1(6) . . . . ?
C3 C4 C19 O3 71.1(5) . . . . ?
C5 C4 C19 O3 -167.6(4) . . . . ?
C14 C8 C9 C11 -6.2(6) . . . . ?
C7 C8 C9 C11 177.0(4) . . . . ?
C14 C8 C9 C10 -134.5(5) . . . . ?
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C7 C8 C14 C13 168.7(5) . . . . ?
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C15 C13 C14 C8 -128.9(5) . . . . ?
C8 C9 C11 C12 39.6(6) . . . . ?
C10 C9 C11 C12 166.3(4) . . . . ?
C10 C5 C6 C7 -60.6(6) . . . . ?
C4 C5 C6 C7 165.4(4) . . . . ?
C14 C8 C7 C6 136.9(5) . . . . ?
C9 C8 C7 C6 -46.2(6) . . . . ?
C5 C6 C7 C8 50.4(6) . . . . ?
O5 C16 C15 O4 -71.7(6) . . . . ?
O5 C16 C15 C13 161.6(5) . . . . ?
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C14 C13 C15 C16 -69.5(6) . . . . ?
C12 C13 C15 C16 173.9(5) . . . . ?
C17 C13 C15 C16 50.8(7) . . . . ?
C9 C11 C12 C13 -61.9(6) . . . . ?
C14 C13 C12 C11 45.2(6) . . . . ?
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  _geom_hbond_angle_DHA

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O1 H1 O4 0.82 1.89 2.674(5) 159.9 2_645
O2 H2 O6 0.82 2.21 2.843(6) 134.4 .
O4 H4 O7 0.82 2.10 2.749(6) 135.5 1_554
O5 H5A O6 0.82 2.49 2.662(6) 93.2 1_554

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_shelxl_version_number 2013-3

_shelx_res_file
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CELL 0.71073 11.7030 6.2643 13.8473 90.000 92.432 90.000
ZERR 2.00 0.0011 0.0006 0.0012 0.000 0.006 0.000
LATT -1
SYMM -X, 0.5+Y, -Z
SFAC C H O
UNIT 40 72 14
OMIT 0 0 1
OMIT -4 6 9
OMIT 7 6 7
OMIT 0 0 2
L.S. 20
ACTA
BOND $H
FMAP 2
PLAN 40
CONF
EQIV $1 X, Y-1, Z
EQIV $2 -X+1, Y-0.5, -Z
EQIV $3 X, Y, Z-1
HTAB O3 O6_$1
HTAB O1 O4_$2
HTAB O2 O6
HTAB O4 O7_$3
HTAB O5 O6_$3
MPLA 5 C8 C9 C11 C13 C14 C12 C17 C15 C16
MPLA 4 C9 C10 C6 C7 C5 C8 C20
MPLA 4 C1 C2 C4 C5 C3 C10 C19 O2 C18 C20
TEMP 21.000
WGHT 0.100000
EXTI 0.097705
FVAR 0.83094
MOLE 1
C3 1 0.280087 0.265339 0.358000 11.00000 0.03837
0.03938 =
0.02782 -0.00453 0.00064 -0.00792
AFIX 13
H3 2 0.272534 0.222409 0.425484 11.00000 -1.20000
AFIX 0
O3 3 0.079264 -0.007026 0.419294 11.00000 0.04587
0.07046 =
0.03533 0.00679 0.00710 -0.00703
AFIX 147

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H3A	2	0.126954	-0.076353	0.451029	11.00000	-1.50000
AFIX	0					
O1	3	0.476743	0.155246	0.370736	11.00000	0.03258
0.06682	=					
		0.03589	-0.00043	-0.00183	0.00829	
AFIX	147					
H1	2	0.528251	0.089083	0.345763	11.00000	-1.50000
AFIX	0					
O2	3	0.321173	0.480082	0.355323	11.00000	0.04652
0.04222	=					
		0.05210	-0.01039	0.00725	-0.00667	
AFIX	147					
H2	2	0.271791	0.561299	0.373999	11.00000	-1.50000
AFIX	0					
C5	1	0.179904	0.284866	0.193813	11.00000	0.03088
0.03852	=					
		0.03178	-0.00185	0.00353	0.00015	
AFIX	13					
H5	2	0.200313	0.436332	0.190475	11.00000	-1.20000
AFIX	0					
C1	1	0.388769	0.192014	0.209272	11.00000	0.03514
0.04742	=					
		0.03085	-0.00336	0.00138	0.00238	
AFIX	23					
H1A	2	0.448376	0.103888	0.183403	11.00000	-1.20000
H1B	2	0.413979	0.339403	0.207332	11.00000	-1.20000
AFIX	0					
C10	1	0.278020	0.167068	0.145143	11.00000	0.03287
0.03351	=					
		0.02767	0.00011	0.00274	-0.00169	
C4	1	0.164563	0.240745	0.303853	11.00000	0.03368
0.04138	=					
		0.02972	-0.00146	0.00104	0.00013	
C18	1	0.082703	0.403856	0.342665	11.00000	0.04013
0.05151	=					
		0.04146	-0.00068	0.00381	0.01016	
AFIX	137					
H18A	2	0.087005	0.400541	0.412035	11.00000	-1.50000
H18B	2	0.006137	0.370819	0.319841	11.00000	-1.50000
H18C	2	0.103087	0.543586	0.320716	11.00000	-1.50000
AFIX	0					
C2	1	0.371555	0.128642	0.313262	11.00000	0.03692
0.05108	=					
		0.02909	0.00187	-0.00348	0.00307	
AFIX	13					
H2A	2	0.348221	-0.021485	0.315257	11.00000	-1.20000
AFIX	0					
C19	1	0.116027	0.017317	0.322345	11.00000	0.04050
0.04884	=					
		0.03357	-0.00516	0.00034	-0.00657	
AFIX	23					
H19A	2	0.051723	-0.008591	0.277362	11.00000	-1.20000
H19B	2	0.174195	-0.088620	0.310365	11.00000	-1.20000
AFIX	0					
C8	1	0.187706	0.287600	-0.016044	11.00000	0.03568
0.03916	=					
		0.03459	0.00872	0.00331	-0.00122	

C9	1	0.297065	0.281003	0.046387	11.00000	0.02966
0.03965 =						
		0.03448	-0.00084	-0.00070	-0.00215	
AFIX	13					
H9	2	0.317183	0.429454	0.061604	11.00000	-1.20000
AFIX	0					
C13	1	0.285680	0.196977	-0.170791	11.00000	0.03680
0.04557 =						
		0.03133	-0.00062	0.00143	-0.00316	
C16	1	0.175289	0.281167	-0.333187	11.00000	0.04113
0.06709 =						
		0.03310	0.00588	0.00380	-0.00066	
AFIX	23					
H16A	2	0.198301	0.160857	-0.371950	11.00000	-1.20000
H16B	2	0.108088	0.240038	-0.298979	11.00000	-1.20000
AFIX	0					
C14	1	0.183359	0.238765	-0.110125	11.00000	0.03720
0.04796 =						
		0.03454	0.00211	0.00467	-0.00006	
AFIX	43					
H14	2	0.111353	0.229684	-0.140939	11.00000	-1.20000
AFIX	0					
O4	3	0.378354	0.357980	-0.310781	11.00000	0.04145
0.06568 =						
		0.03950	-0.00008	0.01063	-0.00796	
AFIX	147					
H4	2	0.404676	0.238321	-0.318917	11.00000	-1.50000
AFIX	0					
C11	1	0.394939	0.189815	-0.008981	11.00000	0.02597
0.06149 =						
		0.03519	0.00554	-0.00005	0.00166	
AFIX	23					
H11A	2	0.466840	0.230922	0.023182	11.00000	-1.20000
H11B	2	0.390406	0.035217	-0.008119	11.00000	-1.20000
AFIX	0					
C6	1	0.067324	0.265204	0.132072	11.00000	0.03424
0.05794 =						
		0.03257	-0.00060	0.00272	-0.00248	
AFIX	23					
H6A	2	0.046734	0.115952	0.124561	11.00000	-1.20000
H6B	2	0.006135	0.337282	0.164145	11.00000	-1.20000
AFIX	0					
C7	1	0.082786	0.365129	0.033244	11.00000	0.03348
0.05206 =						
		0.03772	0.00384	-0.00169	0.00455	
AFIX	23					
H7A	2	0.015764	0.334006	-0.007967	11.00000	-1.20000
H7B	2	0.087610	0.518890	0.040623	11.00000	-1.20000
AFIX	0					
C20	1	0.253574	-0.071342	0.126272	11.00000	0.04737
0.03052 =						
		0.04334	-0.00130	-0.00109	-0.00024	
AFIX	137					
H20A	2	0.324254	-0.145045	0.117284	11.00000	-1.50000
H20B	2	0.204694	-0.086191	0.069222	11.00000	-1.50000
H20C	2	0.216543	-0.131326	0.180552	11.00000	-1.50000
AFIX	0					

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C15   1   0.270991   0.340921  -0.261685   11.00000   0.04767
0.04440 =
        0.03306   0.00137   0.00761  -0.00007
AFIX  13
H15   2   0.253432   0.484439  -0.238366   11.00000  -1.20000
AFIX   0
C12   1   0.393537   0.265629  -0.112675   11.00000   0.03461
0.06130 =
        0.03717  -0.00194   0.00706  -0.00541
AFIX  23
H12A  2   0.460064   0.209195  -0.143450   11.00000  -1.20000
H12B  2   0.398829   0.420144  -0.113476   11.00000  -1.20000
AFIX   0
C17   1   0.290773  -0.040022  -0.198165   11.00000   0.05545
0.04376 =
        0.05837  -0.00404   0.00613  -0.00219
AFIX 137
H17A  2   0.308904  -0.123341  -0.141379   11.00000  -1.50000
H17B  2   0.348637  -0.061057  -0.244344   11.00000  -1.50000
H17C  2   0.217965  -0.083981  -0.225902   11.00000  -1.50000
AFIX   0
O5    3   0.149540   0.457789  -0.393401   11.00000   0.05248
0.09347 =
        0.05837   0.03554   0.00083  -0.00830
AFIX 147
H5A   2   0.153492   0.422116  -0.450137   11.00000  -1.50000
AFIX   0
O7    3   0.431650   0.041930   0.560988   11.00000   0.05342
0.06785 =
        0.04179   0.00222   0.00393   0.01723
O6    3   0.252742   0.756666   0.505052   11.00000   0.06593
0.05822 =
        0.04638   0.00285   0.00113  -0.00124
HKLF  4

REM  AL4_0m in P2(1)
REM  R1 = 0.0757 for 3145 Fo > 4sig(Fo) and 0.1009 for all 4183
data
REM    253 parameters refined using 1 restraints

END

WGHT      0.1181      0.4992

REM Highest difference peak 0.610, deepest hole -0.446, 1-sigma
level 0.128
Q1    1   0.1861  0.2555  0.2392  11.00000  0.05   0.51
Q2    1   0.2433  0.1683  0.2378  11.00000  0.05   0.50
Q3    1   0.2513  0.3244  0.2340  11.00000  0.05   0.47
Q4    1   0.0809  0.2563 -0.2642  11.00000  0.05   0.42
Q5    1   0.1231  0.1807 -0.2258  11.00000  0.05   0.41
Q6    1   0.2001  0.2524 -0.4576  11.00000  0.05   0.40
Q7    1   0.3029  0.2699  0.0958  11.00000  0.05   0.39
Q8    1   0.1179  0.3520 -0.2373  11.00000  0.05   0.39
Q9    1   0.3186  0.1408  0.4093  11.00000  0.05   0.37
Q10   1   0.3652  0.1916 -0.3815  11.00000  0.05   0.36
Q11   1   0.3900  0.3800 -0.2385  11.00000  0.05   0.35
Q12   1   0.3502  0.2910 -0.3710  11.00000  0.05   0.35

```

Q13	1	0.0855	0.2660	0.1079	11.00000	0.05	0.34
Q14	1	0.2261	0.0789	0.2729	11.00000	0.05	0.34
Q15	1	0.4532	0.0809	0.4945	11.00000	0.05	0.34
Q16	1	0.2655	0.3685	0.1632	11.00000	0.05	0.34
Q17	1	0.2758	0.2244	-0.4015	11.00000	0.05	0.34
Q18	1	0.3381	0.2134	-0.2840	11.00000	0.05	0.34
Q19	1	0.2742	0.2239	-0.2112	11.00000	0.05	0.33
Q20	1	0.1277	0.0250	-0.2219	11.00000	0.05	0.32
Q21	1	0.1708	0.4373	-0.2434	11.00000	0.05	0.32
Q22	1	0.1329	0.0156	-0.1992	11.00000	0.05	0.31
Q23	1	0.0842	0.2752	-0.1781	11.00000	0.05	0.31
Q24	1	0.1684	0.1025	-0.2481	11.00000	0.05	0.31
Q25	1	0.1646	0.2465	0.0628	11.00000	0.05	0.31
Q26	1	0.1754	0.2705	-0.2400	11.00000	0.05	0.31
Q27	1	0.3360	0.2944	0.3159	11.00000	0.05	0.31
Q28	1	0.2788	0.1833	-0.0871	11.00000	0.05	0.31
Q29	1	0.0930	0.2640	-0.1536	11.00000	0.05	0.30
Q30	1	0.3957	0.2326	-0.2390	11.00000	0.05	0.30
Q31	1	0.3149	0.2871	0.2760	11.00000	0.05	0.30
Q32	1	0.3712	0.3708	0.2990	11.00000	0.05	0.30
Q33	1	0.2664	0.2764	-0.0391	11.00000	0.05	0.30
Q34	1	0.2430	0.3602	-0.4404	11.00000	0.05	0.30
Q35	1	0.2934	0.4007	-0.3960	11.00000	0.05	0.30
Q36	1	0.2373	0.1148	-0.0653	11.00000	0.05	0.29
Q37	1	0.3239	0.1489	-0.2416	11.00000	0.05	0.29
Q38	1	0.1823	0.1375	-0.1713	11.00000	0.05	0.29
Q39	1	0.2309	0.4428	0.1930	11.00000	0.05	0.29
Q40	1	0.4558	0.3227	-0.2007	11.00000	0.05	0.29

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_shelx_res_checksum 4596

Al-Qubaisi M, Rozita R, Yeap SK, Omar AR, Ali AM, Alitheen NB. 2011. Selective cytotoxicity of goniothalamine against hepatoblastoma HepG2 cells. *Molecules*. 16:2944-2959.

Talupula BK. 2011. Cytotoxicity of PBN spin trap on A204 cells. *J. Advanc. Pharm.Res.* 2:9-17.