Buyiswa G. Hlangothi*, Lungelwa Mahanjana, Eric C. Hosten, Fanie R. van Heerden and Maryna van de Venter

Structural elucidation of 1-(3-acetyl-2,6-dihydroxy-4-methoxyphenyl)-4,5-dihydroxy-2-methylantracene-9,10-dione isolated from *Bulbine latifolia* (L.) Wild, C₂₄H₁₈O₈

$V = 3978.6(3) \text{ \AA}^3$, $Z = 8$, $R_{\text{gt}}(F) = 0.0499$, $wR_{\text{ref}}(F^2) = 0.1320$, $T = 200 \text{ K}$.

CCDC no.: 1837444

One of the four crystallographically independent title molecules is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Orange block
Size:	$0.53 \times 0.47 \times 0.07 \text{ mm}$
Wavelength:	Mo $K\alpha$ radiation ($0.71073 \text{ \AA}$)
μ :	0.11 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	28.4° , $>99\%$
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	36555, 17766, 0.025
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 14484
$N(\text{param})_{\text{refined}}$:	1181
Programs:	Bruker [1], SHELX [2–4], WinGX/ORTEP [5], PLATON [6], Mercury [7]

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Abstract

C₂₄H₁₈O₈, monoclinic, $P2_1$ (no. 4), $a = 7.9654(3) \text{ \AA}$, $b = 23.6910(8) \text{ \AA}$, $c = 21.2314(8) \text{ \AA}$, $\beta = 96.777(2)^\circ$,

***Corresponding author: Buyiswa G. Hlangothi**, Department of Chemistry, Nelson Mandela University, P.O. Box 77000, Port Elizabeth 6031, South Africa, e-mail: Buyiswa.Hlangothi@mandela.ac.za
Lungelwa Mahanjana and Eric C. Hosten: Department of Chemistry, Nelson Mandela University, P.O. Box 77000, Port Elizabeth 6031, South Africa. <https://orcid.org/0000-0003-4173-2550> (E.C. Hosten)

Fanie R. van Heerden: School of Chemistry and Physics, University of KwaZulu-Natal, Private Bag X01, Pietermaritzburg Campus, Pietermaritzburg 3209, Durban, South Africa

Maryna van de Venter: Department of Biochemistry and Microbiology, Nelson Mandela University, P.O. Box 77000, Port Elizabeth 6031, South Africa

Source of material

The plant specimen of *Bulbine latifolia* (L.) Wild was collected from Nelson Mandela University gardens by Lungelwa Mahanjana in February 2014 and was stored in the plant room until the time of extraction. Plant authentication was performed by Dr. Paul Steyn, a botanist at Nelson Mandela University Herbarium, where a specimen of *Bulbine latifolia* (L.) Wild with voucher number PEU24039 has been deposited. The tubers were thoroughly washed with a hard brush to remove dirt and soil particles and then chopped into small pieces. They were then dried in an oven for a week at 40°C until they were completely dry. The dried plant samples were ground into fine powder using an electric mill.

The ground tubers (50 g) of *B. latifolia* were exhaustively extracted with MeOH/CHCl₃ (1:4) by cold maceration at room temperature. The extract was evaporated under reduced pressure to yield a reddish-brown crude extract (11.0 g).

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
O11	−0.0316(7)	0.25062(15)	−0.22112(14)	0.0876(15)
H11	−0.068779	0.283150	−0.230257	0.131 [*]
O12	−0.1123(7)	0.35244(15)	−0.19848(14)	0.0926(16)
O13	−0.1921(9)	0.45747(18)	−0.17954(18)	0.119(2)
H13	−0.173381	0.429302	−0.201701	0.178 [*]
O14	0.0573(4)	0.32213(12)	0.05060(12)	0.0499(7)
O15	−0.2436(3)	0.23125(11)	0.03805(12)	0.0375(6)
H15	−0.325841	0.229569	0.059356	0.056 [*]
O16	−0.3989(3)	0.21237(13)	0.13061(14)	0.0473(7)
O17	0.0312(4)	0.14728(16)	0.22593(13)	0.0570(8)
O18	0.3275(3)	0.18595(15)	0.04826(13)	0.0515(7)
H18	0.410938	0.181214	0.075845	0.077 [*]
O21	0.3543(8)	0.57196(17)	−0.11549(16)	0.1054(18)
H21	0.353816	0.545354	−0.141652	0.158 [*]
O22	0.3550(9)	0.46968(17)	−0.15170(17)	0.113(2)
O23	0.3555(10)	0.36741(19)	−0.19338(17)	0.121(2)
H23	0.336089	0.402222	−0.196229	0.182 [*]
O24	0.4703(5)	0.39538(14)	0.08811(13)	0.0599(8)
O25	0.7305(4)	0.51301(16)	0.13786(14)	0.0574(8)
H25	0.824167	0.507673	0.159640	0.086 [*]
O26	0.9313(3)	0.49251(18)	0.23348(16)	0.0682(10)
O27	0.5304(3)	0.45055(13)	0.32943(12)	0.0427(6)
O28	0.1525(3)	0.48688(17)	0.14285(13)	0.0598(9)
H28	0.082568	0.486026	0.169503	0.090 [*]
O31	−0.0630(5)	0.21561(12)	0.63132(12)	0.0520(7)
H31	−0.036940	0.240780	0.658585	0.078 [*]
O32	−0.0281(5)	0.31812(12)	0.66707(12)	0.0569(8)
O33	0.0097(7)	0.42052(15)	0.70750(15)	0.0834(13)
H33	−0.009416	0.385773	0.709981	0.125 [*]
O34	0.1162(4)	0.38255(12)	0.43671(13)	0.0527(8)
O35	0.2738(3)	0.26875(15)	0.38392(12)	0.0500(7)
H35	0.354935	0.272078	0.362272	0.075 [*]
O36	0.4182(3)	0.28441(19)	0.28772(14)	0.0679(11)
O37	−0.0337(3)	0.33412(12)	0.19092(11)	0.0395(6)
O38	−0.3033(3)	0.29964(16)	0.37554(12)	0.0532(8)
H38	−0.389047	0.302211	0.348573	0.080 [*]
O41	0.4737(5)	0.53365(13)	0.72964(13)	0.0562(8)
H41	0.492979	0.500440	0.742348	0.084 [*]
O42	0.5036(5)	0.42735(13)	0.71254(13)	0.0627(9)
O43	0.4570(7)	0.31857(14)	0.68929(17)	0.0827(13)
H43	0.452093	0.348230	0.710679	0.124 [*]
O44	0.7189(3)	0.45947(12)	0.48904(12)	0.0428(6)
O45	0.2774(3)	0.56433(10)	0.46052(11)	0.0314(5)
H45	0.193566	0.566959	0.432702	0.047 [*]
O46	0.1175(3)	0.58438(11)	0.35651(12)	0.0381(6)
O47	0.5589(3)	0.63485(14)	0.29130(13)	0.0513(7)
O48	0.8734(3)	0.56851(13)	0.47944(14)	0.0485(7)
H48	0.870903	0.537520	0.498533	0.073 [*]
C101	0.0326(4)	0.22279(15)	−0.02676(15)	0.0325(7)
C102	0.0456(5)	0.17867(15)	−0.07115(17)	0.0364(8)
C103	0.0757(6)	0.11851(16)	−0.05031(19)	0.0459(9)
H10A	0.052038	0.093374	−0.086946	0.069 [*]
H10B	0.001023	0.108970	−0.018371	0.069 [*]
H10C	0.193796	0.113953	−0.032037	0.069 [*]
C104	0.0291(6)	0.19077(16)	−0.13510(18)	0.0455(9)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H104	0.046052	0.161481	−0.164252	0.055 [*]
C105	−0.0114(7)	0.24417(19)	−0.15803(18)	0.0551(11)
C106	−0.0298(6)	0.28883(17)	−0.11547(17)	0.0449(9)
C107	−0.0814(7)	0.34465(19)	−0.14012(19)	0.0569(12)
C108	−0.0990(7)	0.39091(18)	−0.09614(19)	0.0521(10)
C109	−0.1528(8)	0.4450(2)	−0.1183(2)	0.0691(15)
C110	−0.1681(9)	0.4882(2)	−0.0747(3)	0.0752(16)
H110	−0.208358	0.524232	−0.089044	0.090 [*]
C111	−0.1252(10)	0.4785(2)	−0.0112(2)	0.0824(19)
H111	−0.134927	0.508408	0.018020	0.099 [*]
C112	−0.0678(7)	0.42625(18)	0.0116(2)	0.0612(13)
H112	−0.036420	0.420669	0.055750	0.073 [*]
C113	−0.0568(6)	0.38213(16)	−0.03082(17)	0.0427(9)
C114	0.0043(5)	0.32637(15)	−0.00514(16)	0.0361(7)
C115	−0.0003(5)	0.27733(15)	−0.04947(15)	0.0360(7)
C116	0.0394(4)	0.20743(15)	0.04123(15)	0.0315(7)
C117	0.1841(4)	0.18686(16)	0.07652(16)	0.0351(7)
C118	0.1849(5)	0.16658(18)	0.13832(17)	0.0415(9)
H118	0.286195	0.152117	0.160595	0.050 [*]
C119	0.0388(5)	0.16757(17)	0.16685(16)	0.0372(8)
C120	0.1801(8)	0.1236(4)	0.2591(3)	0.101(3)
H12A	0.217183	0.091537	0.235073	0.152 [*]
H12B	0.156242	0.110703	0.300995	0.152 [*]
H12C	0.269419	0.152243	0.264111	0.152 [*]
C121	−0.1125(4)	0.18991(14)	0.13514(15)	0.0302(7)
C122	−0.2715(4)	0.19222(15)	0.16205(17)	0.0355(7)
C123	−0.2935(5)	0.1725(2)	0.22775(19)	0.0506(10)
H12D	−0.407467	0.182156	0.237329	0.076 [*]
H12E	−0.209663	0.191064	0.258422	0.076 [*]
H12F	−0.277855	0.131544	0.230402	0.076 [*]
C124	−0.1062(4)	0.20941(14)	0.07184(15)	0.0293(6)
C201	0.4150(4)	0.51458(16)	0.07078(17)	0.0365(8)
C202	0.3967(5)	0.57272(17)	0.05537(18)	0.0432(9)
C203	0.4008(7)	0.6168(2)	0.1066(2)	0.0606(12)
H20A	0.379045	0.654037	0.087270	0.091 [*]
H20B	0.512286	0.616754	0.131727	0.091 [*]
H20C	0.313863	0.608306	0.134262	0.091 [*]
C204	0.3748(6)	0.58944(19)	−0.0070(2)	0.0548(11)
H204	0.361929	0.628464	−0.016629	0.066 [*]
C205	0.3709(8)	0.5509(2)	−0.0560(2)	0.0648(14)
C206	0.3866(6)	0.49291(18)	−0.04296(19)	0.0512(10)
C207	0.3784(8)	0.4528(2)	−0.0954(2)	0.0681(15)
C208	0.3967(7)	0.39271(19)	−0.0828(2)	0.0535(11)
C209	0.3906(8)	0.3531(2)	−0.1321(2)	0.0670(14)
C210	0.4138(7)	0.2961(2)	−0.1180(2)	0.0639(13)
H210	0.411841	0.269346	−0.151456	0.077 [*]
C211	0.4393(6)	0.27833(19)	−0.0567(2)	0.0559(11)
H211	0.453969	0.239215	−0.047846	0.067 [*]
C212	0.4444(6)	0.31668(18)	−0.0064(2)	0.0488(10)
H212	0.460102	0.303837	0.036289	0.059 [*]
C213	0.4261(5)	0.37344(17)	−0.01984(18)	0.0420(9)
C214	0.4367(5)	0.41352(17)	0.03494(17)	0.0402(8)
C215	0.4104(5)	0.47506(16)	0.02136(16)	0.0376(8)
C216	0.4437(4)	0.49852(15)	0.13950(16)	0.0328(7)
C217	0.6043(4)	0.49794(16)	0.17197(18)	0.0370(8)
C218	0.6402(4)	0.48180(15)	0.23664(16)	0.0332(7)

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C219	0.8140(4)	0.48031(17)	0.26578(19)	0.0411(8)
C220	0.8665(4)	0.46511(19)	0.33341(19)	0.0441(9)
H22A	0.820607	0.427953	0.342283	0.066*
H22B	0.823271	0.493392	0.361071	0.066*
H22C	0.990216	0.463990	0.341317	0.066*
C221	0.4993(4)	0.46688(15)	0.26840(16)	0.0320(7)
C222	0.3907(4)	0.43634(18)	0.36285(17)	0.0408(8)
H22D	0.314924	0.468904	0.363073	0.061*
H22E	0.432411	0.425944	0.406587	0.061*
H22F	0.329057	0.404433	0.341822	0.061*
C223	0.3379(4)	0.46970(17)	0.23724(16)	0.0359(8)
H223	0.243913	0.461274	0.259307	0.043*
C224	0.3119(4)	0.48486(17)	0.17352(17)	0.0376(8)
C301	−0.0063(4)	0.26989(14)	0.44886(15)	0.0291(6)
C302	−0.0377(5)	0.21291(16)	0.46279(16)	0.0370(8)
C303	−0.0572(7)	0.16948(18)	0.41074(19)	0.0537(11)
H30A	−0.154521	0.179222	0.380005	0.081*
H30B	−0.075217	0.132257	0.428928	0.081*
H30C	0.045319	0.168681	0.389396	0.081*
C304	−0.0500(5)	0.19638(16)	0.52447(18)	0.0417(8)
H304	−0.067579	0.157664	0.533350	0.050*
C305	−0.0372(5)	0.23504(15)	0.57344(17)	0.0375(8)
C306	−0.0008(4)	0.29194(14)	0.56167(14)	0.0306(7)
C307	0.0040(5)	0.33308(15)	0.61296(16)	0.0371(8)
C308	0.0452(5)	0.39190(15)	0.60106(16)	0.0361(7)
C309	0.0476(6)	0.43288(17)	0.64897(19)	0.0491(10)
C310	0.0928(6)	0.48818(17)	0.6371(2)	0.0511(10)
H310	0.095210	0.515848	0.669542	0.061*
C311	0.1341(5)	0.50268(15)	0.57822(18)	0.0397(8)
H311	0.166085	0.540447	0.570435	0.048*
C312	0.1299(4)	0.46300(15)	0.52982(17)	0.0356(7)
H312	0.158963	0.473586	0.489334	0.043*
C313	0.0830(4)	0.40800(14)	0.54097(15)	0.0294(6)
C314	0.0749(4)	0.36764(15)	0.48761(15)	0.0319(7)
C315	0.0197(4)	0.30816(14)	0.49858(15)	0.0274(6)
C316	−0.0109(4)	0.28635(14)	0.38081(14)	0.0292(6)
C317	0.1310(4)	0.28593(15)	0.34965(15)	0.0311(7)
C318	0.1294(4)	0.30152(15)	0.28427(15)	0.0297(7)
C319	0.2839(4)	0.29940(18)	0.25526(17)	0.0403(8)
C320	0.2970(5)	0.3141(2)	0.18779(18)	0.0491(10)
H32A	0.216763	0.291151	0.160089	0.074*
H32B	0.412193	0.306502	0.178079	0.074*
H32C	0.270797	0.354141	0.180810	0.074*
C321	−0.0304(4)	0.31782(14)	0.25198(14)	0.0287(6)
C322	−0.1936(5)	0.34819(17)	0.15657(16)	0.0389(8)
H32D	−0.178835	0.356156	0.112273	0.058*
H32E	−0.239819	0.381611	0.175592	0.058*
H32F	−0.271805	0.316439	0.158334	0.058*
C323	−0.1731(4)	0.31657(15)	0.28211(15)	0.0308(7)
H323	−0.279322	0.326310	0.259616	0.037*
C324	−0.1626(4)	0.30101(15)	0.34585(15)	0.0323(7)
C401	0.5644(4)	0.55531(14)	0.54196(15)	0.0287(6)
C402	0.5219(4)	0.60098(15)	0.57991(17)	0.0350(7)
C403	0.5049(5)	0.65997(15)	0.55344(19)	0.0421(8)
H40A	0.481270	0.686188	0.586988	0.063*
H40B	0.411938	0.661171	0.518841	0.063*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H40C	0.610467	0.670925	0.537257	0.063*
C404	0.4947(5)	0.59203(15)	0.64212(16)	0.0372(8)
H404	0.467630	0.623128	0.667311	0.045*
C405	0.5062(5)	0.53820(16)	0.66860(16)	0.0379(8)
C406	0.5458(4)	0.49213(14)	0.63208(16)	0.0329(7)
C407	0.5328(5)	0.43450(16)	0.65651(17)	0.0408(8)
C408	0.5414(5)	0.38659(15)	0.61359(17)	0.0372(8)
C409	0.5024(6)	0.33146(17)	0.6321(2)	0.0529(11)
C410	0.5066(7)	0.28751(18)	0.5886(2)	0.0596(12)
H410	0.475315	0.250484	0.599860	0.072*
C411	0.5552(6)	0.29725(18)	0.5299(2)	0.0545(11)
H411	0.559845	0.266661	0.501248	0.065*
C412	0.5979(5)	0.35090(16)	0.51160(19)	0.0416(8)
H412	0.633254	0.357038	0.470964	0.050*
C413	0.5884(4)	0.39563(14)	0.55313(16)	0.0319(7)
C414	0.6346(4)	0.45287(14)	0.53310(16)	0.0326(7)
C415	0.5800(4)	0.50157(13)	0.56895(15)	0.0284(6)
C416	0.5713(4)	0.56792(14)	0.47305(15)	0.0283(6)
C417	0.4182(4)	0.57638(13)	0.43482(15)	0.0265(6)
C418	0.4109(4)	0.59695(14)	0.37165(15)	0.0287(6)
C419	0.2446(4)	0.59968(14)	0.33347(16)	0.0316(7)
C420	0.2224(5)	0.6189(3)	0.2667(2)	0.0588(13)
H42A	0.246614	0.659371	0.265028	0.088*
H42B	0.105703	0.611846	0.248139	0.088*
H42C	0.300158	0.598122	0.242645	0.088*
C421	0.5668(4)	0.61137(16)	0.34984(16)	0.0353(7)
C422	0.7119(6)	0.6523(3)	0.2687(2)	0.0761(18)
H42D	0.767794	0.680730	0.297371	0.114*
H42E	0.686611	0.668440	0.226111	0.114*
H42F	0.786788	0.619617	0.266888	0.114*
C423	0.7197(4)	0.60250(17)	0.38665(17)	0.0380(8)
H423	0.823301	0.612202	0.371317	0.046*
C424	0.7182(4)	0.57901(15)	0.44671(17)	0.0359(8)

The extract was subjected to column chromatography (VLC: column size: 80 X 4) on silica gel (300 g) eluting with *n*-hexane containing increasing amounts of ethyl acetate to afford 12 major fractions ca. 200 mL each. Based on TLC profile, similar compounds were identified in the fractions; therefore the fractions were combined to yield two main fractions, fraction one and fraction two. Fraction one was chromatographed using column chromatography with the solvent system of 15% ethyl acetate in *n*-hexane and the collected fractions yielded yellow-orange crystals upon evaporation.

¹H NMR (CDCl₃, 25 °C) δ (400 MHz, ppm): 14.10 (s, 1H, OH-2'), 12.52 (s, 1H, OH-1), 11.88 (s, 1H, OH-8), 7.51 (m, *J* = 7.9 Hz, 1H, H-6), 7.53 (m, *J* = 7.8 Hz, 1H, H-5), 7.22 (s, 1H, H-2), 7.17 (d, *J* = 5.6 Hz, 1H, H-7), 6.08 (s, 1H, H-5'), 3.88 (s, 3H, OCH₃), 2.59 (s, 3H, CO—CH₃), 2.09 (s, 3H, CH₃). **¹³C NMR** (chloroform, 23 °C) δ (126 MHz, ppm): 203.7 (CO), 192.7 (C-9), 182.7 (C-10), 163.3 (C-2'), 163.2 (C-1), 162.9 (C-4'), 161.9 (C-8), 159.3 (C-6'), 152.4 (C-3), 137.1 (C-6), 134.4 (C-5a), 132.9 (C-4a), 125.8

(C-4), 125.0 (C-2), 123.9 (C-7), 120.1 (C-5), 115.4 (C-8a), 115.3 (C-1a), 107.1 (C-1'), 106.2 (C-3'), 90.5 (C-5'), 55.6 (C—OCH₃), 33.1 (C—COCH₃), 21.0 (C—CH₃). **IR**: 3381 cm⁻¹ (O—H), 2921 cm⁻¹ (C—H), 1599 cm⁻¹ (C=C), **Mp** 239–242 °C.

Experimental details

Absolute configuration was established by anomalous-dispersion effects in diffraction measurements {Flack parameter: 0.0(2)} on the crystal. Carbon-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with $U_{\text{iso}}(\text{H})$ set to $1.2U_{\text{eq}}(\text{C})$. The H atoms of the methyl groups were allowed to rotate with a fixed angle around the C—C bonds to best fit the experimental electron density (HFIX 137 in the SHELXL program [3]), with $U_{\text{iso}}(\text{H})$ set to $1.5U_{\text{eq}}(\text{C})$. The H atoms of the hydroxyl groups were allowed to rotate with a fixed angle around the C—O bonds to best fit the experimental electron density (HFIX 147 in the SHELXL program [3]), with $U_{\text{iso}}(\text{H})$ set to $1.5U_{\text{eq}}(\text{O})$.

Comment

The genus *Bulbine* Wolf (family Xanthorrhoeaceae and subfamily Asphodeloideae) comprises approximately 80 species mainly confined to southern Africa and Australia [8, 9]. In South Africa, the species have a centre of diversity in the Greater Cape Region where some of the 46 southern Africa species occur including *B. latifolia* [10]. *B. latifolia* (*B. natalensis*) known as rooiwortel (Afrikaans), ibhucu (Zulu) and ingcwelwane (isiXhosa) is a frost-tender evergreen plant with a rosette of fleshy, thornless, yellow-green leaves and is well distributed in the Eastern and Northern parts of South Africa as well as in other parts of Africa such as Malawi, Zimbabwe and Mozambique [11]. The roots have been used to ease vomiting and diarrhoea and also to treat convulsions, venereal disease, diabetes, rheumatism, urinary complaints and blood disorders [12].

Previous phytochemical investigations of this plant resulted in isolation of anthraquinones and phytosterols [13, 14]. In the present study, isolation of knipholone from the tubers of *B. latifolia* and the crystal structure of the compound are reported. Knipholone is the common name for 1-(3-acetyl-2,6-dihydroxy-4-methoxyphenyl)-4,5-dihydroxy-2-methylantraquinone and has been reported as a marker for the *bulbine* species. But, the detailed crystal data of knipholone has not been reported previously. We have successfully obtained single crystals of knipholone and its structure was unambiguously determined.

The asymmetric unit cell contains four molecules of knipholone with all bond lengths and angles in expected

ranges and similar to those of a related compound [15]. Although knipholone does not contain a chiral center, it is chiral due to restricted rotation about the biaryl axis. All four molecules in the asymmetric unit cell have the same stereochemistry corresponding to the (P)-1 stereostructure [10]. Each molecule has a slightly different conformation with the smallest and largest RMSD between two molecules being 0.2339 and 0.6266 respectively. One of the molecules has an dihedral angle of 67.92(9)° between the least square planes formed by the anthraquinone group and the phenyl ring. The dihedral angles for the remaining three molecules are almost orthogonal varying from 88.05(7) to 89.41(8)°. The RMS deviation of the least square plane through the anthraquinone group also shows large variation from 0.030 to 0.288.

Extensive intra and inter-molecular hydrogen bonding of the type O—H...O occurs. All the hydroxyl groups on the 1,8-dihydroxyanthraquinone groups have an interaction with the nearby carbonyl oxygen with a graph set descriptor [16] of S1,1(6). Similarly there is the same S1,1(6) interaction between a hydroxyl and acetyl group on the phenyl rings of all four knipholone molecules. For three of the knipholone molecules the remaining phenyl hydroxyl groups are involved in inter-molecular interactions. On one of the molecules the remaining phenyl hydroxyl has an intra-molecular interaction with a carbonyl oxygen on its anthraquinone group with graph set descriptor of S1,1(8) and bond length 2.879(4) Å. This enhances the distortion of the anthraquinone group which has the largest planar RMSD of all four molecules. There are three sets of intermolecular hydrogen bond interactions with graph set descriptors of C1,1(8) linking adjacent molecules in infinite chains. Two adjacent dihydroxyanthraquinone groups interact to form a ring structure with a R2,2(16) descriptor. In addition there are four discrete intermolecular interaction patterns with D3,3 descriptors and atom numbers of 23, 25, 21 and 26.

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