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Crystal structure of {tetraqua-bis(1-(4-hydroxy-2-oxotetrahydrofuran-3-yl)-2-((4*aS*,6*R*,8*aS*)-6-hydroxy-5-(hydroxymethyl)-5,8*a*-dimethyl-2-methylenedecahydronaphthalen-1-yl)ethane-1-sulfonato- k^2O,O') calcium(II)}-{triaqua-bis(1-(4-hydroxy-2-oxotetrahydrofuran-3-yl)-2-((4*aS*,6*R*,8*aS*)-6-hydroxy-5-(hydroxymethyl)-5,8*a*-dimethyl-2-methylenedecahydronaphthalen-1-yl)ethane-1-sulfonato- k^2O,O') calcium(II)} – water – acetone (1/1/8/2)

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Abstract

$C_{43}H_{78}CaO_{22}S_2$, monoclinic, $P2_1$ (no. 4), $a = 18.2539(3)$ Å, $b = 15.3118(3)$ Å, $c = 18.3718(4)$ Å, $\beta = 91.2637(17)^\circ$, $Z = 4$, $V = 5133.65(18)$ Å³, $R_{gt}(F) = 0.0544$, $wR_{ref}(F^2) = 0.1622$, $T = 293(2)$ K.

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Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

Andrographolide calcium bisulfite crude product was provided by Jiangsu Jiuxu Pharmaceutical Com. Ltd. To begin with, the raw materials were dissolved in mixture of absolute water and acetone and then slow evaporation at room temperature for 3 days. Finally, we obtained the crystals of the title compound.

Experimental details

All hydrogen atoms were located in calculated positions and refined as riding atoms. The hydrogen atoms of tertiary and secondary carbons for isotropic displacement factors $U_{iso}(H)$ were set to 1.2 times $U_{eq}(C)$, 1.5 times $U_{eq}(C)$ of methyl hydrogen atoms and 1.5 times $U_{eq}(O)$.

Comment

Andrographolide, a diterpenoid lactone, can be obtained from the extract of traditional herb *Andrographis paniculata*

Table 1: Data collection and handling.

Crystal:	Colourless
Size:	$0.22 \times 0.16 \times 0.13$ mm
Wavelength:	Cu $K\alpha$ radiation (1.54184 Å)
μ :	2.48 mm^{-1}
Diffractometer, scan mode:	Xcalibur, ω
θ_{max} , completeness:	70.9° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	25633, 15314, 0.027
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 12706
$N(\text{param})_{\text{refined}}$:	1271
Programs:	Bruker [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1185 (3)	0.3018 (3)	0.7137 (3)	0.0319 (10)
H1A	0.0834	0.2837	0.6762	0.038*
H1B	0.1625	0.2671	0.7083	0.038*
C1"	0.6199 (3)	0.5511 (3)	0.2148 (3)	0.0326 (10)
H1"A	0.5870	0.5296	0.1768	0.039*
H1"B	0.6662	0.5206	0.2106	0.039*
C1'	−0.1129 (2)	0.2983 (3)	1.2771 (2)	0.0309 (10)
H1'A	−0.0771	0.2789	1.3134	0.037*
H1'B	−0.1571	0.2643	1.2832	0.037*
C1A	0.3838 (3)	0.5465 (3)	0.7801 (2)	0.0312 (10)
H1AA	0.4216	0.5291	0.8151	0.037*
H1AB	0.3407	0.5113	0.7888	0.037*
C2	0.0864 (3)	0.2838 (3)	0.7888 (3)	0.0396 (11)
H2A	0.0738	0.2224	0.7926	0.048*
H2B	0.1227	0.2971	0.8265	0.048*
C2"	0.5876 (3)	0.5312 (3)	0.2889 (3)	0.0395 (11)
H2"A	0.5795	0.4688	0.2932	0.047*
H2"B	0.6222	0.5485	0.3271	0.047*
C2'	−0.0830 (3)	0.2809 (3)	1.2010 (3)	0.0382 (11)
H2'A	−0.0718	0.2193	1.1961	0.046*
H2'B	−0.1200	0.2959	1.1644	0.046*
C2A	0.4103 (3)	0.5281 (4)	0.7036 (3)	0.0429 (12)
H2AA	0.4226	0.4666	0.6993	0.051*
H2AB	0.3714	0.5410	0.6684	0.051*
C3	0.0185 (3)	0.3389 (4)	0.8001 (2)	0.0357 (11)
H3	−0.0167	0.3253	0.7606	0.043*
C3"	0.5160 (3)	0.5788 (4)	0.2988 (2)	0.0361 (11)
H3"	0.4825	0.5612	0.2592	0.043*
C3'	−0.0144 (3)	0.3341 (4)	1.1884 (2)	0.0358 (11)
H3'	0.0219	0.3181	1.2261	0.043*
C3A	0.4771 (3)	0.5829 (4)	0.6870 (2)	0.0410 (12)
H3A	0.5152	0.5686	0.7235	0.049*
C4	0.0339 (3)	0.4375 (3)	0.7977 (2)	0.0342 (10)
C4"	0.5241 (3)	0.6787 (3)	0.2957 (3)	0.0363 (11)
C4'	−0.0270 (2)	0.4330 (3)	1.1931 (2)	0.0324 (10)
C4A	0.4630 (3)	0.6813 (4)	0.6916 (2)	0.0356 (11)
C5	0.0685 (2)	0.4548 (3)	0.7212 (2)	0.0286 (9)
H5	0.0307	0.4357	0.6860	0.034*

with extraordinary efficacy for treating various diseases including diarrhea, hepatic protection, rheumatoid arthritis, upperrespiratory tract infection, cancer and so on [4–7], and the Andrographolide's contribution of these effects had been proved by pharmacological researches [8]. Furthermore, Andrographolide is a neuroprotection regulator in central nervous system (CNS) [9]. Andrographolide has been identified an anti-inflammatory, anti-bacteria and anti-virus drug, however, which blocks its excellent clinically application prospect for extremely poor water solubility and low bioavailability. Given inadequacies of Andrographolide, researchers improved its solubility by introducing hydrophilic sodium bisulfite group, resulting in Andrographolide sodium bisulfite (ASB). In a recent study, we found Andrographolide calcium bisulfite (ACB) which is a related impurity of ASB.

The asymmetric unit contains four andrographolide bisulfite anions, two calcium cations, two molecules of acetone and 14 molecules of water. Ca1 adopts a distorted polyhedron geometry by coordinating to four oxygen atoms of hydroxyl from a pair of organic ligands and four oxygen atoms of four water ligands (see the figure). In contrast Ca1a is sevenfold coordinated by four hydroxy groups of two organic ligands and three water ligands.

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
C5"	0.5599 (2)	0.6993 (3)	0.2204 (2)	0.0310 (10)
H5"	0.5244	0.6776	0.1839	0.037*
C5'	−0.0607 (2)	0.4507 (3)	1.2700 (2)	0.0288 (9)
H5'	−0.0226	0.4313	1.3048	0.035*
C5A	0.4329 (2)	0.6991 (3)	0.7696 (2)	0.0298 (9)
H5A	0.4724	0.6799	0.8028	0.036*
C6	0.0795 (3)	0.5522 (3)	0.7042 (3)	0.0389 (11)
H6A	0.1185	0.5754	0.7352	0.047*
H6B	0.0349	0.5840	0.7144	0.047*
C6"	0.5655 (3)	0.7978 (3)	0.2050 (3)	0.0432 (12)
H6"A	0.6022	0.8236	0.2373	0.052*
H6"B	0.5188	0.8255	0.2144	0.052*
C6'	−0.0705 (3)	0.5474 (3)	1.2871 (3)	0.0387 (11)
H6'A	−0.1101	0.5710	1.2570	0.046*
H6'B	−0.0260	0.5788	1.2757	0.046*
C6A	0.4237 (3)	0.7963 (3)	0.7866 (3)	0.0406 (11)
H6AA	0.3830	0.8198	0.7579	0.049*
H6AB	0.4677	0.8276	0.7734	0.049*
C7	0.0989 (3)	0.5650 (4)	0.6239 (3)	0.0432 (12)
H7A	0.0577	0.5480	0.5928	0.052*
H7B	0.1093	0.6262	0.6149	0.052*
C7"	0.5863 (3)	0.8134 (4)	0.1251 (3)	0.0432 (12)
H7"A	0.5470	0.7935	0.0929	0.052*
H7"B	0.5934	0.8754	0.1169	0.052*
C7'	−0.0877 (3)	0.5606 (4)	1.3674 (3)	0.0428 (12)
H7'A	−0.0460	0.5429	1.3975	0.051*
H7'B	−0.0972	0.6219	1.3766	0.051*
C7A	0.4095 (3)	0.8096 (4)	0.8680 (3)	0.0452 (13)
H7AA	0.4524	0.7921	0.8964	0.054*
H7AB	0.4003	0.8709	0.8774	0.054*
C8	0.1648 (3)	0.5107 (3)	0.6059 (2)	0.0331 (10)
C8"	0.6555 (3)	0.7649 (3)	0.1089 (2)	0.0344 (10)
C8'	−0.1537 (3)	0.5073 (3)	1.3864 (2)	0.0316 (9)
C8A	0.3448 (3)	0.7565 (3)	0.8899 (2)	0.0334 (10)
C9	0.1524 (2)	0.4139 (3)	0.6189 (2)	0.0258 (8)
H9	0.1074	0.3980	0.5921	0.031*
C9"	0.6483 (2)	0.6672 (3)	0.1210 (2)	0.0267 (9)
H9"	0.6041	0.6490	0.0937	0.032*
C9'	−0.1419 (2)	0.4104 (3)	1.3739 (2)	0.0266 (9)
H9'	−0.0958	0.3950	1.3989	0.032*
C9A	0.3551 (2)	0.6598 (3)	0.8769 (2)	0.0246 (8)
H9AA	0.4015	0.6434	0.9011	0.030*
C10	0.1374 (2)	0.3989 (3)	0.7024 (2)	0.0253 (9)
C10"	0.6325 (2)	0.6496 (3)	0.2037 (2)	0.0257 (9)
C10'	−0.1301 (2)	0.3953 (3)	1.2901 (2)	0.0246 (8)
C10A	0.3648 (2)	0.6436 (3)	0.7925 (2)	0.0257 (9)
C11	0.2138 (2)	0.3555 (3)	0.5897 (2)	0.0336 (10)
H11A	0.2604	0.3746	0.6106	0.040*
H11B	0.2056	0.2959	0.6054	0.040*
C11"	0.7115 (2)	0.6126 (3)	0.0911 (2)	0.0338 (10)
H11E	0.7049	0.5520	0.1049	0.041*
H11F	0.7573	0.6328	0.1127	0.041*
C11'	−0.2015 (2)	0.3523 (3)	1.4063 (2)	0.0303 (9)
H11C	−0.1944	0.2925	1.3906	0.036*
H11D	−0.2492	0.3714	1.3882	0.036*
C11A	0.2948 (2)	0.6020 (3)	0.9101 (2)	0.0310 (9)

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
H11G	0.2473	0.6218	0.8922	0.037*
H11H	0.3014	0.5422	0.8940	0.037*
C12	0.2179 (2)	0.3576 (3)	0.5063 (2)	0.0320 (10)
H12	0.2224	0.4190	0.4919	0.038*
C12"	0.7156 (2)	0.6188 (3)	0.0076 (2)	0.0317 (10)
H12"	0.7200	0.6806	−0.0054	0.038*
C12'	−0.1999 (2)	0.3559 (3)	1.4902 (2)	0.0299 (9)
H12'	−0.1897	0.4165	1.5041	0.036*
C12A	0.2964 (2)	0.6045 (3)	0.9938 (2)	0.0299 (9)
H12A	0.3078	0.6646	1.0083	0.036*
C13	0.1501 (3)	0.3217 (4)	0.4679 (2)	0.0386 (11)
C13"	0.6494 (2)	0.5829 (4)	−0.0319 (2)	0.0348 (11)
C13'	−0.1414 (3)	0.3005 (4)	1.5257 (3)	0.0415 (12)
C13A	0.3531 (3)	0.5471 (4)	1.0289 (3)	0.0357 (11)
C14	0.1208 (3)	0.2437 (5)	0.4696 (3)	0.0563 (15)
H14	0.1396	0.1969	0.4963	0.068*
C14"	0.6164 (3)	0.5071 (5)	−0.0270 (3)	0.0503 (14)
H14"	0.6312	0.4621	0.0040	0.060*
C14'	−0.1386 (4)	0.2157 (5)	1.5393 (3)	0.0597 (16)
H14'	−0.1745	0.1758	1.5250	0.072*
C14A	0.3521 (3)	0.4620 (4)	1.0451 (3)	0.0520 (14)
H14A	0.3133	0.4244	1.0345	0.062*
C15	0.0541 (4)	0.2406 (6)	0.4235 (4)	0.069 (2)
H15A	0.0594	0.1995	0.3838	0.083*
H15B	0.0119	0.2242	0.4517	0.083*
C15"	0.5523 (3)	0.5030 (6)	−0.0779 (4)	0.0650 (19)
H15E	0.5577	0.4563	−0.1130	0.078*
H15F	0.5073	0.4941	−0.0517	0.078*
C15'	−0.0705 (4)	0.1931 (7)	1.5804 (5)	0.095 (3)
H15C	−0.0816	0.1699	1.6280	0.114*
H15D	−0.0420	0.1504	1.5542	0.114*
C15A	0.4218 (4)	0.4364 (6)	1.0822 (4)	0.077 (2)
H15G	0.4129	0.4143	1.1306	0.092*
H15H	0.4469	0.3919	1.0546	0.092*
C16	0.1040 (4)	0.3769 (6)	0.4219 (4)	0.073 (2)
C16"	0.6087 (4)	0.6348 (6)	−0.0861 (4)	0.070 (2)
C16'	−0.0736 (4)	0.3380 (6)	1.5559 (4)	0.071 (2)
C16A	0.4243 (3)	0.5808 (5)	1.0549 (3)	0.0564 (16)
C17	0.2271 (3)	0.5462 (4)	0.5866 (3)	0.0444 (13)
H17A	0.2314	0.6067	0.5837	0.053*
H17B	0.2669	0.5109	0.5759	0.053*
C17"	0.7168 (3)	0.8051 (4)	0.0924 (3)	0.0481 (13)
H17E	0.7183	0.8658	0.0905	0.058*
H17F	0.7586	0.7728	0.0827	0.058*
C17'	−0.2156 (3)	0.5431 (4)	1.4072 (3)	0.0458 (13)
H17C	−0.2195	0.6035	1.4104	0.055*
H17D	−0.2553	0.5079	1.4185	0.055*
C17A	0.2842 (3)	0.7938 (4)	0.9125 (3)	0.0464 (13)
H17G	0.2810	0.8543	0.9149	0.056*
H17H	0.2446	0.7595	0.9259	0.056*
C18	−0.0390 (3)	0.4863 (5)	0.8016 (3)	0.0560 (16)
H18A	−0.0667	0.4772	0.7573	0.084*
H18B	−0.0297	0.5475	0.8080	0.084*
H18C	−0.0662	0.4647	0.8420	0.084*
C18"	0.4472 (3)	0.7177 (5)	0.2960 (3)	0.065 (2)
H18G	0.4203	0.6927	0.3352	0.098*

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H18H	0.4225	0.7051	0.2506	0.098*
H18I	0.4505	0.7798	0.3025	0.098*
C18'	0.0481 (3)	0.4777 (5)	1.1904 (3)	0.0536 (15)
H18D	0.0416	0.5386	1.1797	0.080*
H18E	0.0767	0.4511	1.1532	0.080*
H18F	0.0730	0.4715	1.2367	0.080*
C18A	0.5369 (3)	0.7292 (5)	0.6843 (3)	0.0592 (17)
H18J	0.5621	0.7069	0.6430	0.089*
H18K	0.5663	0.7201	0.7276	0.089*
H18L	0.5281	0.7906	0.6779	0.089*
C19	0.0853 (3)	0.4683 (4)	0.8602 (3)	0.0408 (12)
H19A	0.1275	0.4299	0.8633	0.049*
H19B	0.1027	0.5266	0.8495	0.049*
C19"	0.5699 (3)	0.7154 (4)	0.3598 (3)	0.0464 (13)
H19E	0.6138	0.6802	0.3662	0.056*
H19F	0.5851	0.7744	0.3481	0.056*
C19'	-0.0761 (3)	0.4670 (3)	1.1313 (2)	0.0365 (10)
H19C	-0.1186	0.4293	1.1261	0.044*
H19D	-0.0933	0.5250	1.1437	0.044*
C19A	0.4102 (3)	0.7129 (4)	0.6309 (2)	0.0394 (11)
H19G	0.3677	0.6748	0.6287	0.047*
H19H	0.3934	0.7713	0.6424	0.047*
C20	0.2071 (2)	0.4226 (3)	0.7465 (2)	0.0331 (10)
H20A	0.2491	0.3989	0.7230	0.050*
H20B	0.2042	0.3987	0.7947	0.050*
H20C	0.2116	0.4850	0.7495	0.050*
C20"	0.6996 (3)	0.6786 (4)	0.2493 (2)	0.0362 (11)
H20G	0.6944	0.6596	0.2987	0.054*
H20H	0.7034	0.7411	0.2481	0.054*
H20I	0.7430	0.6533	0.2296	0.054*
C20'	-0.2000 (2)	0.4209 (3)	1.2474 (2)	0.0329 (10)
H20D	-0.2026	0.4833	1.2433	0.049*
H20E	-0.2421	0.3999	1.2726	0.049*
H20F	-0.1991	0.3954	1.1997	0.049*
C20A	0.2934 (2)	0.6685 (3)	0.7525 (2)	0.0318 (10)
H20J	0.2916	0.6410	0.7055	0.048*
H20K	0.2913	0.7307	0.7466	0.048*
H20L	0.2525	0.6493	0.7803	0.048*
Ca1	0.00043 (6)	0.34412 (7)	0.99371 (6)	0.0317 (2)
Ca1A	0.49034 (5)	0.58920 (7)	0.49181 (5)	0.0345 (2)
O1	-0.0148 (2)	0.3157 (3)	0.86785 (19)	0.0495 (10)
H1	-0.051 (3)	0.282 (4)	0.8592 (13)	0.074*
O1"	0.4842 (2)	0.5523 (3)	0.36639 (19)	0.0494 (10)
H1"	0.450 (3)	0.515 (4)	0.3584 (14)	0.074*
O1'	0.0151 (2)	0.3109 (3)	1.11907 (19)	0.0498 (10)
H1'	0.050 (3)	0.275 (4)	1.1256 (13)	0.075*
O1A	0.5044 (2)	0.5585 (3)	0.61679 (19)	0.0596 (13)
H1AC	0.542 (3)	0.525 (4)	0.6229 (13)	0.089*
O2	0.0489 (2)	0.4688 (3)	0.92948 (18)	0.0449 (9)
H2	0.065 (3)	0.514 (2)	0.9527 (14)	0.067*
O2"	0.5310 (2)	0.7165 (3)	0.42693 (19)	0.0491 (9)
H2"	0.533 (3)	0.7685 (12)	0.444 (2)	0.074*
O2'	-0.0390 (2)	0.4708 (2)	1.06272 (17)	0.0389 (8)
H2'	-0.050 (3)	0.5197 (15)	1.0433 (15)	0.058*
O2A	0.4443 (2)	0.7138 (3)	0.56072 (18)	0.0442 (9)
H2AC	0.427 (3)	0.758 (2)	0.5383 (14)	0.066*

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
O3	0.0469 (3)	0.3288 (5)	0.3965 (3)	0.096 (2)
O3"	0.5527 (3)	0.5872 (5)	-0.1130 (3)	0.0843 (17)
O3'	-0.0325 (3)	0.2736 (6)	1.5865 (3)	0.101 (2)
O3A	0.4638 (3)	0.5151 (5)	1.0855 (3)	0.0828 (18)
O4	0.1095 (4)	0.4524 (5)	0.4072 (4)	0.127 (3)
O4"	0.6209 (4)	0.7075 (5)	-0.1064 (4)	0.116 (3)
O4'	-0.0538 (3)	0.4126 (5)	1.5550 (4)	0.110 (2)
O4A	0.4481 (3)	0.6530 (5)	1.0514 (3)	0.093 (2)
O5	0.2895 (2)	0.2110 (3)	0.4973 (2)	0.0547 (10)
O5"	0.7888 (2)	0.4726 (3)	-0.0010 (2)	0.0497 (9)
O5'	-0.3022 (2)	0.2396 (3)	1.5038 (2)	0.0514 (10)
O5A	0.1884 (2)	0.4931 (3)	1.0031 (2)	0.0532 (10)
O6	0.2979 (2)	0.3132 (3)	0.3967 (2)	0.0514 (10)
O6"	0.7939 (2)	0.5735 (3)	-0.10293 (19)	0.0487 (9)
O6'	-0.2805 (2)	0.3379 (3)	1.60480 (19)	0.0498 (10)
O6A	0.2139 (2)	0.5863 (3)	1.10723 (19)	0.0510 (10)
O7	0.3607 (2)	0.3415 (3)	0.5112 (2)	0.0551 (11)
O7"	0.85846 (19)	0.6054 (3)	0.0098 (2)	0.0519 (10)
O7'	-0.3406 (2)	0.3889 (3)	1.4940 (2)	0.0554 (11)
O7A	0.1583 (2)	0.6459 (3)	0.9971 (2)	0.0583 (12)
O8	0.1273 (2)	0.3110 (5)	1.0020 (3)	0.088 (2)
H8A	0.1373	0.2552	1.0085	0.132*
H8B	0.1534	0.3414	1.0407	0.132*
O8A	0.3616 (2)	0.5747 (4)	0.4684 (3)	0.0828 (17)
H8AA	0.3758	0.5252	0.4821	0.124*
H8AB	0.3506	0.5806	0.4212	0.124*
O9	-0.0060 (2)	0.1870 (3)	0.9931 (3)	0.0615 (12)
H9A	0.0242	0.1531	1.0316	0.092*
H9B	-0.0582	0.1580	0.9878	0.092*
O9A	0.4922 (3)	0.4324 (3)	0.4928 (3)	0.0651 (12)
H9AB	0.5341	0.4083	0.4717	0.098*
H9AC	0.4526	0.4073	0.4673	0.098*
O10	-0.12636 (19)	0.3260 (3)	0.9881 (3)	0.0545 (10)
H10A	-0.1449	0.3688	0.9655	0.082*
H10B	-0.1399	0.2696	0.9941	0.082*
O10A	0.61798 (18)	0.5681 (3)	0.4985 (2)	0.0475 (9)
H10C	0.6453	0.6058	0.4674	0.071*
H10D	0.6335	0.5102	0.4853	0.071*
S1	0.29810 (6)	0.30140 (9)	0.47466 (7)	0.0347 (3)
S1"	0.79544 (6)	0.56290 (10)	-0.02483 (6)	0.0328 (3)
S1'	-0.28769 (6)	0.32806 (9)	1.52647 (6)	0.0330 (3)
S1A	0.20726 (6)	0.57929 (10)	1.02853 (6)	0.0358 (3)
C21	0.7993 (5)	0.6146 (5)	0.6792 (4)	0.074 (2)
C22	0.7951 (6)	0.5534 (7)	0.6155 (5)	0.110 (4)
H22A	0.7720	0.4999	0.6299	0.165*
H22B	0.8436	0.5412	0.5992	0.165*
H22C	0.7669	0.5798	0.5767	0.165*
C23	0.7288 (5)	0.6368 (7)	0.7128 (5)	0.100 (3)
H23A	0.7212	0.6988	0.7102	0.150*
H23B	0.7299	0.6187	0.7628	0.150*
H23C	0.6896	0.6074	0.6872	0.150*
O11	0.8569 (4)	0.6453 (5)	0.7008 (3)	0.097 (2)
C21A	0.6926 (4)	0.3687 (5)	0.8209 (4)	0.0679 (18)
C22A	0.7650 (5)	0.3973 (6)	0.7937 (5)	0.088 (2)
H22D	0.7675	0.3852	0.7425	0.131*
H22E	0.8034	0.3662	0.8192	0.131*

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
H22F	0.7709	0.4589	0.8017	0.131*
C23A	0.6926 (6)	0.3011 (7)	0.8801 (5)	0.105 (3)
H23D	0.6434	0.2923	0.8961	0.157*
H23E	0.7228	0.3206	0.9203	0.157*
H23F	0.7115	0.2471	0.8617	0.157*
O11A	0.6358 (3)	0.3990 (5)	0.7973 (3)	0.096 (2)
O14	0.2371 (5)	0.5421 (5)	0.3628 (4)	0.133 (3)
H14B	0.1965	0.5325	0.3832	0.199*
H14C	0.2450	0.5175	0.3192	0.199*
O19	0.6069 (4)	0.4479 (5)	0.6579 (3)	0.117 (3)
H19I	0.6489	0.4437	0.6392	0.175*
H19J	0.6053	0.4191	0.7037	0.175*
O15	0.2159 (4)	0.7090 (5)	0.2986 (3)	0.113 (2)
H15I	0.2252	0.6640	0.3271	0.169*
H15J	0.2438	0.7470	0.3335	0.169*
O16	0.2711 (4)	0.4682 (5)	0.2127 (4)	0.125 (3)
H16A	0.2493	0.5097	0.1904	0.187*
H16B	0.2659	0.4280	0.1792	0.187*
O12	0.8746 (3)	0.7059 (5)	0.8383 (3)	0.0848 (18)
H12B	0.8579	0.7120	0.7951	0.127*
H12C	0.8478	0.6664	0.8566	0.127*
O17	0.2466 (4)	0.3092 (5)	0.1245 (4)	0.122 (3)
H17I	0.2346	0.2942	0.1656	0.183*
H17J	0.2794	0.2718	0.1148	0.183*
O13	0.3789 (4)	0.4407 (5)	0.3225 (4)	0.117 (3)
H13A	0.3527	0.4550	0.2856	0.175*
H13B	0.3559	0.3986	0.3416	0.175*
O18	0.1169 (3)	0.7024 (4)	0.1821 (3)	0.0770 (15)
H18M	0.1336	0.7078	0.2254	0.115*
H18N	0.1502	0.6665	0.1705	0.115*

The organic ligand andrographolide calcium bisulfite consists of two fused cyclohexanes adopting chair conformations and a nearly planar five-membered lactonic ring. Ca–O distances are in the range of those observed in reported Ca(II) complexes [10, 11]. The O–S distances coincided with the normal ranges. And bond angles around the central Ca (II) ion vary from 71.47 (13)° to 164.85 (19)°. The Flack parameter (absolute configuration) was determined to 0.003(7), thus the configuration at atoms C3, C4, C5, C9, C10 and C12 are in *R*, *R*, *S*, *R*, *S* and *R*, respectively.

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