Qin Luo, Qing-Guo Meng, Gui-Ge Hou, Sheng Jiang, Yong-Sheng Jin and Yue Gao*

Crystal structure of (8*R*,10*R*,14*R*,*Z*)-12-hydroxy-2-((6-methoxypyridin-2-yl)methylene)-4,4,8,10,14-pentamethyl-17-((*R*)-2,6,6-trimethyltetrahydro-2*H*-pyran-2-yl)hexadecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one–water (2/1), C₃₇H₅₆NO_{4.5}

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.12 × 0.10 × 0.08 mm
Wavelength:	Cu Kα radiation (1.54178 Å)
μ:	0.59 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω
θ _{max} , completeness:	73.6°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	14308, 6554, 0.046
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 5487
<i>N</i> (<i>param</i>) _{refined} :	612
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Abstract

C₃₇H₅₆NO_{4.5}, tetragonal, *P*₄2₁2/c (no. 92), *a* = 10.4368(10) Å, *b* = 10.4268(10) Å, *c* = 61.5166(11) Å, *V* = 6700.80(18) Å³, *Z* = 8, *R*_{gt}(*F*) = 0.0557, *wR*_{ref}(*F*²) = 0.1350, *T* = 100 K.

CCDC no.: 2089133

The molecular structure 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.

Source of material

(8*R*,10*R*,14*R*)-12-Hydroxy-4,4,8,10,14-pentamethyl-17-((*R*)-2,6,6-trimethyltetrahydro-2*H*-pyran-2-yl)hexadecahydro-3*H*-cyclopenta[*a*]phenanthren-3-one (100 mg, 0.22 mmol) and 6-methoxy-2-pyridinecarboxaldehyde (30.0 mg, 0.22 mmol) were dissolved in 1.4 mL methanol. After adding 0.72 mL of 25% NaOH aqueous solution, the reaction system was opalescent. The reaction system was stirred at room temperature for 5 h. The response endpoint was detected by thin layer chromatography (TLC). When the reaction was stopped, a moderate amount of water was

<https://doi.org/10.1515/ncrs-2021-0284>

Received July 13, 2021; accepted August 29, 2021;
published online September 7, 2021

*Corresponding author: Yue Gao, Department of Lab Teaching, School of Pharmacy, Naval Medical University, Shanghai, 200433, P.R. China, E-mail: gaoyue2000@hotmail.com

Qin Luo and Qing-Guo Meng, School of Pharmacy, Collaborative Innovation Center of Advanced Drug Delivery System and Biotech Drugs in Universities of Shandong, Key Laboratory of Molecular Pharmacology and Drug Evaluation (Yantai University), Ministry of Education, Yantai University, Yantai, P.R. China. <https://orcid.org/0000-0003-4684-8923> (Q. Luo)

Gui-Ge Hou, School of Pharmacy, The Key Laboratory of Prescription Effect and Clinical Evaluation of State Administration of Traditional Chinese Medicine of China, Binzhou Medical University, Yantai, 264003, P.R. China. <https://orcid.org/0000-0002-9493-3981>

Sheng Jiang, Shandong Wendeng Jizhen American Ginseng Industry Co., Ltd., Shandong, 264400, P.R. China

Yong-Sheng Jin, Department of Organic Chemistry, School of Pharmacy, Naval Medical University, Shanghai, 200433, P.R. China

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}
O1 ^a	0.0487 (4)	0.2764 (5)	0.52841 (7)	0.0287 (11)
H1 ^a	−0.019314	0.307386	0.524310	0.043*
O1 ^b	0.0368 (4)	0.1529 (5)	0.52199 (7)	0.0314 (12)
H1 ^b	−0.033400	0.174839	0.517318	0.047*
O2	0.6118 (3)	−0.0279 (4)	0.61718 (5)	0.0736 (12)
O3 ^a	−0.1901 (5)	0.3522 (5)	0.52263 (9)	0.0250 (11)
O3 ^b	−0.2106 (9)	0.1794 (8)	0.51019 (11)	0.030 (2)
O4	0.3865 (3)	0.5363 (3)	0.55606 (5)	0.0557 (8)
N1	0.4692 (3)	0.3783 (3)	0.57838 (4)	0.0297 (6)
C1	0.3573 (3)	0.1239 (3)	0.58524 (4)	0.0214 (6)
H1A	0.381442	0.153712	0.570877	0.026*
H1B	0.299619	0.186981	0.591428	0.026*
C2	0.4756 (3)	0.1174 (3)	0.59910 (4)	0.0235 (6)
C3	0.5028 (3)	−0.0033 (4)	0.61148 (5)	0.0381 (9)
C4	0.3924 (4)	−0.0907 (3)	0.61793 (5)	0.0377 (9)
C5	0.2665 (3)	−0.0598 (3)	0.60592 (5)	0.0313 (8)
H5A ^b	0.221451	0.004934	0.614558	0.038*
H5B ^a	0.229698	0.011163	0.614269	0.038*
C6 ^b	0.1938 (11)	−0.1821 (12)	0.60828 (18)	0.026 (2)
H6A ^b	0.193562	−0.210965	0.623269	0.032*
H6B ^b	0.230150	−0.248853	0.599198	0.032*
C6 ^a	0.1512 (9)	−0.1606 (11)	0.60396 (19)	0.026 (2)
H6'A ^a	0.177938	−0.228886	0.594282	0.031*
H6'B ^a	0.137180	−0.198347	0.618173	0.031*
C7 ^b	0.0590 (11)	−0.1472 (10)	0.60080 (14)	0.027 (2)
H7A ^b	0.024788	−0.081482	0.610319	0.032*
H7B ^b	0.004327	−0.222053	0.602043	0.032*
C7 ^a	0.0238 (10)	−0.1084 (9)	0.59579 (14)	0.027 (2)
H7'A ^a	−0.007572	−0.046295	0.606238	0.033*
H7'B ^a	−0.037344	−0.178341	0.595331	0.033*
C8 ^b	0.0552 (8)	−0.0980 (8)	0.57699 (12)	0.0184 (15)
C8 ^a	0.0273 (8)	−0.0442 (8)	0.57315 (12)	0.0216 (16)
C9 ^b	0.1552 (13)	0.0108 (9)	0.5750 (2)	0.017 (2)
H9 ^b	0.119666	0.080640	0.583752	0.021*
C9 ^a	0.1427 (12)	0.0529 (9)	0.5729 (2)	0.018 (2)
H9 ^a	0.117468	0.118354	0.583498	0.021*
C10	0.2842 (3)	−0.0035 (3)	0.58280 (5)	0.0266 (7)
C11 ^b	0.1552 (8)	0.0644 (8)	0.55145 (13)	0.0214 (17)
H11A ^b	0.217508	0.133201	0.550453	0.026*
H11B ^b	0.181509	−0.002792	0.541521	0.026*
C11 ^a	0.1489 (7)	0.1265 (8)	0.55135 (14)	0.0222 (16)
H11C ^a	0.223226	0.182361	0.551366	0.027*
H11D ^a	0.158198	0.066365	0.539428	0.027*
C12 ^b	0.0246 (6)	0.1149 (7)	0.54451 (10)	0.0231 (13)
H12 ^b	0.003447	0.190426	0.553267	0.028*
C12 ^a	0.0284 (6)	0.2060 (7)	0.54803 (9)	0.0241 (13)
H12 ^a	0.018435	0.265792	0.560192	0.029*
C13 ^b	−0.0788 (6)	0.0146 (6)	0.54766 (9)	0.0201 (12)
H13 ^b	−0.057066	−0.057228	0.538074	0.024*
C13 ^a	−0.0853 (5)	0.1160 (6)	0.54738 (8)	0.0207 (13)
H13 ^a	−0.069965	0.055564	0.535475	0.025*
C14 ^b	−0.0779 (7)	−0.0392 (8)	0.57149 (10)	0.0208 (14)
C14 ^a	−0.0973 (6)	0.0349 (8)	0.56874 (9)	0.0206 (13)
C15 ^b	−0.1914 (6)	−0.1319 (6)	0.57022 (10)	0.0248 (14)
H15A ^b	−0.226368	−0.147749	0.584574	0.030*

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H15B ^b	−0.165082	−0.212906	0.563911	0.030*
C15 ^a	−0.2222 (7)	−0.0394 (7)	0.56373 (11)	0.0285 (14)
H15C ^a	−0.203838	−0.115446	0.555215	0.034*
H15D ^a	−0.264253	−0.065156	0.577098	0.034*
C16 ^b	−0.2912 (7)	−0.0650 (6)	0.55563 (10)	0.0259 (14)
H16A ^b	−0.360629	−0.031153	0.564386	0.031*
H16B ^b	−0.326506	−0.125349	0.545242	0.031*
C16 ^a	−0.3077 (6)	0.0537 (7)	0.55078 (11)	0.0302 (15)
H16C ^a	−0.379259	0.081804	0.559638	0.036*
H16D ^a	−0.341211	0.011738	0.537911	0.036*
C17 ^b	−0.2203 (6)	0.0465 (6)	0.54347 (10)	0.0220 (13)
H17 ^b	−0.239396	0.125914	0.551328	0.026*
C17 ^a	−0.2232 (6)	0.1705 (6)	0.54420 (9)	0.0230 (13)
H17 ^a	−0.235938	0.236705	0.555283	0.028*
C18 ^b	0.0861 (7)	−0.2141 (7)	0.56226 (10)	0.0253 (14)
H18A ^b	0.169509	−0.246741	0.565821	0.038*
H18B ^b	0.084820	−0.187729	0.547307	0.038*
H18C ^b	0.023218	−0.279912	0.564500	0.038*
C18 ^a	0.0429 (7)	−0.1505 (7)	0.55607 (11)	0.0307 (15)
H18D ^a	0.121650	−0.195580	0.558595	0.046*
H18E ^a	0.044361	−0.113128	0.541808	0.046*
H18F ^a	−0.027686	−0.209187	0.557119	0.046*
C19	0.3641 (4)	−0.0901 (3)	0.56776 (6)	0.0427 (10)
H19A	0.358775	−0.058838	0.553113	0.064*
H19B	0.331433	−0.176037	0.568363	0.064*
H19C	0.451861	−0.089516	0.572425	0.064*
C20 ^b	−0.2670 (6)	0.0649 (6)	0.51962 (10)	0.0255 (14)
C20 ^a	−0.2572 (6)	0.2295 (7)	0.52252 (10)	0.0228 (13)
C21 ^b	−0.2625 (7)	0.3083 (7)	0.51346 (12)	0.0296 (15)
C21 ^a	−0.2228 (6)	0.4608 (7)	0.50916 (10)	0.0287 (14)
C22 ^b	−0.4087 (8)	0.3092 (10)	0.51373 (16)	0.0303 (19)
H22A ^b	−0.440266	0.301944	0.498957	0.036*
H22B ^b	−0.438373	0.390191	0.519594	0.036*
C22 ^a	−0.3666 (6)	0.4819 (7)	0.50904 (10)	0.0339 (16)
H22C ^a	−0.388009	0.543840	0.497870	0.041*
H22D ^a	−0.392652	0.517134	0.522947	0.041*
C23 ^b	−0.4632 (7)	0.1997 (7)	0.52735 (11)	0.0295 (15)
H23A ^b	−0.437503	0.209427	0.542415	0.035*
H23B ^b	−0.556085	0.200592	0.526694	0.035*
C23 ^a	−0.4400 (7)	0.3586 (9)	0.50488 (12)	0.0365 (17)
H23C ^a	−0.531294	0.375435	0.505533	0.044*
H23D ^a	−0.419999	0.326880	0.490447	0.044*
C24 ^b	−0.4132 (6)	0.0763 (7)	0.51848 (11)	0.0313 (15)
H24A ^b	−0.439896	0.068179	0.503440	0.038*
H24B ^b	−0.451012	0.005960	0.526539	0.038*
C24 ^a	−0.4049 (7)	0.2589 (9)	0.52157 (13)	0.0263 (16)
H24C ^a	−0.450440	0.180224	0.518288	0.032*
H24D ^a	−0.432958	0.288003	0.535764	0.032*
C25 ^b	−0.2218 (7)	−0.0410 (7)	0.50468 (9)	0.0311 (16)
H25A ^b	−0.261083	−0.031147	0.490675	0.047*
H25B ^b	−0.245263	−0.122554	0.510718	0.047*
H25C ^b	−0.130333	−0.036640	0.503184	0.047*
C25 ^a	−0.2177 (15)	0.1499 (15)	0.50306 (18)	0.032 (3)
H25D ^a	−0.264797	0.177448	0.490488	0.049*
H25E ^a	−0.235796	0.061227	0.505864	0.049*
H25F ^a	−0.127648	0.160510	0.500475	0.049*

Table 2: (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C26 ^b	−0.2075 (8)	0.3678 (8)	0.53420 (16)	0.0372 (18)
H26A ^b	−0.244289	0.326551	0.546666	0.056*
H26B ^b	−0.227363	0.457591	0.534545	0.056*
H26C ^b	−0.116160	0.356621	0.534384	0.056*
C26 ^a	−0.1540 (7)	0.5707 (7)	0.51987 (12)	0.0389 (17)
H26D ^a	−0.181017	0.577572	0.534744	0.058*
H26E ^a	−0.173794	0.648842	0.512345	0.058*
H26F ^a	−0.063253	0.555921	0.519358	0.058*
C27 ^b	−0.2119 (8)	0.3812 (8)	0.49376 (14)	0.0435 (19)
H27A ^b	−0.119980	0.379206	0.493797	0.065*
H27B ^b	−0.240727	0.468483	0.494380	0.065*
H27C ^b	−0.243267	0.341792	0.480696	0.065*
C27 ^a	−0.1712 (7)	0.4422 (9)	0.48588 (11)	0.0413 (18)
H27D ^a	−0.085139	0.409851	0.486514	0.062*
H27E ^a	−0.171711	0.522868	0.478388	0.062*
H27F ^a	−0.224527	0.382256	0.478253	0.062*
C28	0.4374 (6)	−0.2307 (4)	0.61539 (7)	0.0728 (17)
H28A	0.439185	−0.252966	0.600247	0.109*
H28B	0.379208	−0.286541	0.622906	0.109*
H28C	0.521695	−0.239815	0.621424	0.109*
C29	0.3740 (4)	−0.0638 (4)	0.64256 (5)	0.0405 (9)
H29A	0.449087	−0.090514	0.650345	0.061*
H29B	0.300994	−0.110608	0.647791	0.061*
H29C	0.360414	0.026194	0.644774	0.061*
C30 ^b	−0.1175 (10)	0.0690 (8)	0.58766 (19)	0.027 (2)
H30A ^b	−0.123582	0.034313	0.602081	0.040*
H30B ^b	−0.199102	0.103454	0.583436	0.040*
H30C ^b	−0.054314	0.135796	0.587423	0.040*
C30 ^a	−0.1313 (9)	0.1246 (9)	0.58818 (17)	0.025 (2)
H30D ^a	−0.160802	0.074003	0.600214	0.038*
H30E ^a	−0.197559	0.183146	0.583854	0.038*
H30F ^a	−0.056578	0.171986	0.592441	0.038*
C31	0.5602 (3)	0.2131 (4)	0.60169 (5)	0.0313 (8)
H31	0.627148	0.194916	0.611165	0.038*
C32	0.5645 (3)	0.3409 (4)	0.59210 (5)	0.0326 (8)
C33	0.4794 (4)	0.4935 (3)	0.56961 (6)	0.0413 (9)
C34	0.5805 (5)	0.5780 (4)	0.57309 (8)	0.0587 (13)
H34	0.584061	0.656908	0.566091	0.070*
C35	0.6739 (5)	0.5406 (4)	0.58714 (8)	0.0645 (15)
H35	0.741805	0.595335	0.590243	0.077*
C36	0.6681 (4)	0.4205 (4)	0.59686 (6)	0.0515 (12)
H36	0.732004	0.393666	0.606355	0.062*
C37	0.2867 (4)	0.4481 (4)	0.55072 (7)	0.0533 (11)
H37A	0.248291	0.416382	0.563834	0.080*
H37B	0.321910	0.377810	0.542606	0.080*
H37C	0.222944	0.490767	0.542116	0.080*
O5	0.2546 (2)	0.2546 (2)	0.500000	0.0464 (10)
H5C ^c	0.278688	0.186144	0.493598	0.070*
H5D ^c	0.196893	0.229105	0.508802	0.070*

^aOccupancy: 0.507 (3), ^bOccupancy: 0.493 (3), ^cOccupancy: 0.5.

added to the container and the mixture was extracted with ethyl acetate (twice). The combined organic phase was washed with saturated sodium chloride solution, dried with anhydrous sodium sulfate, filtered, reduced pressure

concentration, yellow solid is obtained. The crude product was purified by silica-gel thin layer chromatography (petroleum ether: ethyl acetate = 3/1, v/v). The single crystal of the target compound was obtained by recrystallization with ethyl acetate solution.

Experimental details

The H atoms were placed in idealized positions and treated as riding on their parent atoms, with $d(C-H) = 0.97 \text{ \AA}$ (methylene), $d(C-H) = 0.93 \text{ \AA}$ (aromatic), $d(C-H) = 0.96 \text{ \AA}$ (methyl) $d(C-H) = 0.93 \text{ \AA}$ (alkenyl) and $d(O-H) = 0.82 \text{ \AA}$ (−OH). The absolute configuration was derived from the synthesis and the configuration of the educts. Almost the whole organic molecule shows a disorder, which limits the significance of all bond lengths and angles. The figure shows only one of the two overlaid models.

Comment

Ginseng is a traditional Chinese medicinal plant, which has been widely used for the treatment of heart failure [4, 5] and various tissue damages under cellular and environmental stress. Ginseng is effective in improving blood circulation and brain function, enhancing immune function, preventing diabetes, as well as having anti-cancer, anti-inflammatory [6, 7] and antibacterial properties. Ginsenosides are the major active components of ginseng responsible for pharmacological actions. Ginsenosides are divided into two groups according to their glycosidic structures: dammarane and oleanane. There are two types of dammaranes: protopanaxadiol (PD) type [8, 9] and protopanaxatriol type sharing a tetrahydrofuran ring and a dammarane skeleton. Moreover, the conformation of the compound will have a certain influence on the biological activity [10]. Our group has done a lot of research work on panaxadiol derivatives [11] and panaxatriol derivatives [12], and obtained molecular data based on crystal structures [13, 14]. The title compound is a PD derivative. It is possible to modify the structure of ginsenoside which is an important saponin in ginsenoside.

Single-crystal structure analysis reveals that the title compound contains one drug molecule and one half of a water molecule in the asymmetric unit (cf. the Figure). Except for the substituents on C(2), the structure of the title compound is the same as that of panaxadiol. In the crystal structure, the pyridine ring has a planar conformation, and the other six membered rings except the ring with the keto

group which has a chair conformation. The bond lengths and angles are all in the expected ranges.

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: This work was supported by the National Natural Science Foundation of China (No. 81473104, 81773563). Meanwhile, this work was also supported by National Natural Science Foundation of China (Grant no. 81573585) and other Science Foundation (No. 13ZJZ06).

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

References

1. Rigaku OD. CrysAlis^{PRO}; Rigaku Oxford Diffraction Ltd: Yarnton, Oxfordshire, England, 2017.
2. Sheldrick G. M. A short history of *SHELX*. *Acta Crystallogr.* 2008, *A64*, 112–122.
3. Sheldrick G. M. Crystal structure refinement with *SHELXL*. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Streit W. J., Xue Q. S., Tischer J., Bechmann I. Microglial pathology. *Acta Neuropathol. Commun.* 2014, *2*, 142.
5. Wang J. Z., Wang H. Y., Mou X. D., Luan M. Z., Zhang X. F., He X. T., Zhao F. L., Meng Q. G. The advances on the protective effects of ginsenosides on myocardial ischemia and ischemia-reperfusion injury. *Mini Rev. Med. Chem.* 2020, *20*, 1610–1618.
6. Zhang J. Q., Zhang Q., Xu Y. R., Li H. X., Zhao F. L., Wang C. M., Liu Z., Liu P., Liu Y. N., Meng Q. G., Zhao F. Synthesis and *in vitro* anti-inflammatory activity of C20 epimeric ocotillol-type triterpenes and protopanaxadiol. *Planta Med.* 2019, *85*, 292–301.
7. Zhang S. N., Zhao Y. Q. Crystallization separation of anti-tumor constituent 20(R) 25–OCH₃–PPD. *Chin. Tradit. Herb. Drugs* 2014, *45*, 770–773.
8. Liu J., Xu Y. R., Yang J. J., Wang W. Z., Zhang J. Q., Zhang R. M., Meng Q. G. Discovery, semisynthesis, biological activities, and metabolism of ocotillol-type saponins. *J. Ginseng Res.* 2017, *41*, 373–378.
9. Ma Y., Wang H. Y., Zhang X. F., Zhao F. L., Meng Q. G. Crystal structure of (3*S*,8*R*,10*R*,12*R*,14*R*)-12-hydroxy-4,4,8,10,14-pentamethyl-17-((*R*)-2,6,6-trimethyltetrahydro-2*H*-pyran-2-yl) hexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl acetate C₃₂H₅₄O₄. *Z. Kristallogr. N. Cryst. Struct.* 2021, *236*, 163–166.
10. Yang Q. W., Wang N., Zhang J., Chen G., Xu H., Meng Q. G., Du Y., Yang X., Fan H. Y. *In vitro* and *in silico* evaluation of stereoselective effect of ginsenoside isomers on platelet P2Y₁₂ receptor. *Phytomedicine* 2019, *64*, 152889.
11. Wang J. Z., Weng W. Z., Ma Y., He X. T., Meng Q. G. Crystal structure of (1*S*,3*aR*,3*bR*,10*aR*, 10*bR*,12*aR*)-8-amino-3*a*,3*b*,6,6,10*a*-pentamethyl-1-((*S*)-2,6,6-trimethyltetrahydro-2*H*-pyran-2-yl)-2,3,3*a*,3*b*,4,5,5*a*,6,10,10*a*,10*b*,11,12,12*a*-tetradecahydro-1*H*-cyclopenta[7,8]phenanthro[2,3-*d*]thiazol-12-ol - a panaxadiol derivative, C₃₁H₅₀N₂O₂S. *Z. Kristallogr. N. Cryst. Struct.* 2019, *234*, 397–400.
12. Sun K. W., Wang X. H., Ma G. Q., Luo Q., Wang Y. H., Meng Q. G. The crystal structure of (5*R*,8*R*,9*R*,10*R*, 12*R*,13*R*,14*R*)-12-hydroxy-4,4,8,10,14-pentamethyl-17-((*R*)-2,6,6-trimethyltetrahydro-2*H*-pyran-2-yl) tetradecahydro-3*H*-cyclopenta[*a*]phenanthrene-3,6(2*H*)-dione, C₃₀H₄₈O₄. *Z. Kristallogr. N. Cryst. Struct.* 2021, *236*, 17–20.
13. Zhao R. L., Wang H. Y., Luan M. Z., Zheng X., Zhao F. L., Meng Q. G. Crystal structure of (3*H*,5*R*,8*R*,9*R*,10*R*, 12*R*,13*R*,14*R*)-4,4,8,10,14-pentamethyl-17-((*R*)-2,6,6-trimethyltetrahydro-2*H*-pyran-2-yl) hexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,12-diol, C₃₀H₅₂O₃. *Z. Kristallogr. N. Cryst. Struct.* 2020, *235*, 1329–1331.
14. Wang C. M., Liu J., Deng J. Q., Wang J. Z., Weng W. Z., Chu H. X., Meng Q. G. Advances in the chemistry, pharmacological diversity, and metabolism of 20(*R*)-ginseng saponins. *J. Ginseng Res.* 2020, *44*, 14–23.