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Development and Application of Sentinel-2 Canopy Chlorophyll Content (CCC) Validation Dataset of Winter Wheat in Yucheng, Shandong of China

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Abstract: The Sentinel-2 canopy chlorophyll content (CCC) validation dataset of winter wheat in Yucheng, Shandong of China consists of two parts: Canopy Chlorophyll Content observed in field (CCC_{Field} = LAI × LCC) for 107 sample plots were observed in Yucheng, Shandong Province from May 9 to 16, 2020, including LAI and SPAD; and Canopy Chlorophyll Content retrieved from Sentinel-2 satellite ($CCC_{Sentinel}$) with a spatial resolution of 10 m. Five correlation analyses of CCC_{Field} and $CCC_{Sentinel}$ shows that the coefficient of determination (R^2) ranges from 0.889,9 to 0.928,0, with a RMSE of 29.267, which indicates that $CCC_{Sentinel}$ can explain at least 88.99% of the CCC_{Field} variation during the period from late of April to early May. The dataset is archived in .shp, .kmz, .tif and .xlsx data formats, and consists of 18 data files with data size of 215 MB (compressed into three files with 160 MB).

Keywords: chlorophyll content; SPAD; LAI; Sentinel-2; field observation; winter wheat; Yucheng

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Dataset Availability Statement:

The dataset supporting this paper was published and is accessible through the *Digital Journal of Global Change Data Repository* at: https://doi.org/10.3974/geodb.2020.09.14.V1 or https://cstr.escience.org.cn/CSTR:20146.11.2020.09.14.V1.

1 Introduction

Chlorophyll is not only the basis of photosynthesis[1], but also the close relationship with nitrogen level. It can be measured relatively easier, and can be used as a proxy for nitrogen level[2–4]. Chlorophyll content can be expressed by leaf chlorophyll content (LCC) or canopy chlorophyll content (CCC). The measurement methods of chlorophyll content can be divided into ground measurement and remote sensing inversion. The ground measurement of chlorophyll includes laboratory analysis, ground spectrum measurement, leaf color card and

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[2] Wang, Z. X., Li, F. Sentinel-2 canopy chlorophyll content (CCC)validation dataset of winter wheat in Yucheng, Shandong of China [J/DB/OL]. *Digital Journal of Global Change Data Repository*, 2020. https://doi.org/10.3974/geodb.2020.09.14.V1. https://cstr.escience.org.cn/CSTR:20146.11.2020.09.14.V1.

so on[5,6]. The ground method is suitable for measuring chlorophyll content in a small range, and the "mass method" is used for measuring chlorophyll content in many early studies, which cannot be used for remote sensing validation[7,8]. Therefore, some scholars call for using the "area method" in the future measurement of chlorophyll content [2,9,10].

In principle, the method of retrieving chlorophyll content by remote sensing can be divided into statistical method and physical mechanism method[11]. The parameters in the statistical method include not only the common vegetation index, but also the parameters obtained through the specific spectral interval, such as the location of the red edge, the parameters based on synthesis, derivative, and continuum removal[12–18]. The physical mechanism method assumes that there is a causal relationship between the remote sensing data and chlorophyll content. The physical relationship can be used to build a radioactive transfer model (RTM), and the "look-up table (LUT)" method can be used to retrieve chlorophyll content[19,20]. In theory, physical mechanism method has higher "portability" than statistical method, but its performance still needs to be verified. For instance, some research shows that physical mechanism method is also affected by seasonality [20] and vegetation type[21–23].

At present, there are three chlorophyll content products retrieved by remote sensing on the global scale: (1) the MERIS-LCC product (2002–2012) was developed by University of Toronto, Canada, 300 m, weekly[24]; (2) MODIS-LCC product, 500m-8d, was developed by Chinese scholars[25]; (3) Sentinel-CCC product is developed by ESA, but it requires users to download Sentinel-2 L2A data and process L2A into Sentinel-CCC using SNAP-Biophysical Model, Sentinel-CCC product can be as fine as 10 m with 5-day temporal resolution[26].

Due to the low spatial resolution (300–500 m) of MERIS and MODIS LCC products, it is difficult to obtain reliable ground validation data for CCC with 300–500 m resolution. However, Sentinel-CCC has high spatial resolution (up to 10 m), which can be validated with field survey relatively easier. If 10 m Sentinel-CCC can be validated to meet some criteria with field observation, it may be used to further verify the CCC of 300–500 m resolution. This dataset[27] includes the relative chlorophyll index (SPAD) and LAI of 107 winter wheat plots in Yucheng, Shandong province in May 2020, and the model converted from SPAD to LCC. The spatial resolution of the plots is 10 m, which can be used to verify chlorophyll products with lower spatial resolution after up scaling.

2 Metadata of the Dataset

Metadata of the Sentinel-2 canopy chlorophyll content (CCC) validation dataset of winter wheat in Yucheng, Shandong of China[27] is summarized in Table 1.

3 Methodology

3.1 Study Area

The sampling area is located in Yucheng county, Shandong province, which belongs to the alluvial plain of the lower Yellow River. The altitude range is 17.5–26.1 m, with small fluctuation. The annual average temperature is 13.3 ºC, the annual average precipitation is 555.5 mm, the annual average evaporation is 1,884.8 mm, the frost free period is 202 days, and the annual sunshine is 2,546.2 hours. Winter wheat and maize rotation is the main way of land use, in which winter wheat was sown in October of the previous year and harvested in early June of the present year. The field observation time is from May 9 to 16, 2020 when winter wheat is in the filling stage.

Table 1 Metadata summary of the Sentinel-2 canopy chlorophyll content (CCC) validation dataset of winter wheat in Yucheng, Shandong of China

Items	Descriptions
Dataset full name	Sentinel-2 canopy chlorophyll content (CCC) validation dataset of winter wheat in Yucheng, Shandong of China
Dataset short name	CCC_WinterWheat_Yucheng_2020
Authors	Wang, Z. X. L-5255-2016, Institute of Geographic Sciences and Natural Resources Research, Chinese Academy of Sciences, wangzx@igsnrr.ac.cn Li, F. L-3424-2018, Institute of Geographic Sciences and Natural Resources Research, Chinese Academy of Sciences, lif@igsnrr.ac.cn
Geographic region	Yucheng, Shandong province, China 116°31′17.11″E–116°35′45.48″E; 36°44′59.71″N–36°49′59.81″N
Sampling date	Field work: May 9–16, 2020; Sentinel-2 sensing: July 29, 2020; May 19,2020
Spatial resolution	10 m×10 m
Data format	.shp, .kml, .xlsx, .tif Data size 160 MB
Data files	3 files
Foundation	Ministry of Science and Technology of P. R. China (2016YFA0600201)
Data computing environment	SNAP Biophysical Processor (ESA), ArcMap10.5
Data publisher	Global Change Research Data Publishing & Repository, http://www.geodoi.ac.cn
Address	No. 11A, Datun Road, Chaoyang District, Beijing 100101, China
Data sharing policy	***Data*** from the Global Change Research Data Publishing & Repository includes metadata, datasets (in the *Digital Journal of Global Change Data Repository*), and publications (in the *Journal of Global Change Data & Discovery*). ***Data*** sharing policy includes: (1) ***Data*** are openly available and can be free downloaded via the Internet; (2) End users are encouraged to use ***Data*** subject to citation; (3) Users, who are by definition also value-added service providers, are welcome to redistribute ***Data*** subject to written permission from the GCdataPR Editorial Office and the issuance of a ***Data*** redistribution license; and (4) If ***Data*** are used to compile new datasets, the 'ten per cent principal' should be followed such that ***Data*** records utilized should not surpass 10% of the new dataset contents, while sources should be clearly noted in suitable places in the new dataset[28]
Communication and searchable system	DOI, CSTR, Crossref, DCI, CSCD, CNKI, SciEngine, WDS/ISC, GEOSS

3.2 The Principles of Validation Data Development

The aim of collecting validation data is to validate the canopy chlorophyll content products of Sentinel-2, with a spatial resolution of 10 m and a temporal resolution of 5 days. Therefore, the field observation and data processing follow the following principles.

(1) Spatial resolution: the spatial positioning accuracy of field observation should be better than 10 m.

(2) Temporal resolution: the time of field observation data and Sentinel-2 data should match on 1-day scale. Because of the great variation of winter wheat in each growth period, the ideal verification should be that the satellite sensing and the field survey are on the same day. However, due to various restrictions, such time consistency is rare. The processing principle of time consistency is: Taking the field observation time as the benchmark, using the latest high-quality satellite data, and assuming that the CCC changes linearly during the two satellite sensing periods, using the principle of inverse time interval weight, the satellite data is interpolated into the data corresponding to the field observation time.

The satellite data product to be verified: the canopy chlorophyll content of Sentinel-2 ($CCC_{Sentinel}$).

Canopy chlorophyll content is the sum of all the leaf chlorophyll content (LCC), determined by equation (1) and (2).

$$CCC_{Field} = LAI \times LCC \tag{1}$$

where LAI is leaf area index, observed by LAI-2200 in the field; LCC is leaf chlorophyll density (μg/cm^2), which is determined by field SPAD and an empirical equation. Here, we use an equation from Zhuge town of Luoyang, Henan province in April 2019.

$$LCC = 0.0188 \times SPAD^{2.0033},\ R^2 = 0.768 \tag{2}$$

In addition, if there is no LCC available, the LAI×SPAD of field measurement may also approximately verify the $CCC_{Sentinel}$, which is defined as:

$$CCC_{Field} = LAI \times SPAD \tag{3}$$

3.3 Implementation of Field Observation

The field observation includes two items (LAI and SPAD) and follows four steps: sampling design; determine the actual spatial location of sample plot; pretreatment of sample plot before observation; and field observation.

3.3.1 Sampling Design (Homework, in Advance)

Based on these Sentinel-2 CCC products, we can preliminarily select sample plots, make them into KML files, import them into mobile GPS tools, and use them as field navigation maps. CCC classification map and preliminary plot distribution map can also be printed for field survey.

3.3.2 Determine the Actual Spatial Location of Sample Plot

The location of pre-set sample plot maybe inaccurate and needs to be adjusted according to more detailed field information. Generally, "parcel" is the basic unit of field observation. Each parcel belongs to a farmer. The crop varieties and crop management in this parcel are relatively consistent, but the differences between plots are relatively large. In this case, the plot is usually long in the north-south direction and short in the east-west direction. For example, the parcel size of a typical family is 2,220 m^2, which is equivalent to 100 m × 22.2 m, or 80 m × 27.75 m. The narrow side of the parcel is usually 20–30 m, while the spatial resolution of Sentinel-2 is 10 m. Consider the spatial matching error between the satellite and the ground, we should choose the sample plot with smaller CCC difference between adjacent parcels.

3.3.3 Pretreatment of Sample Plot Before Observation

3.3.3.1 Sample Plot Preparation for LAI

In order to yield LAI accurately with LAI-2200 instrument, the time interval between A and B measurements should be as short as possible. Therefore, before the measurement, we need to be well-prepared to avoid the interference of unexpected events. The sample plot pretreatment for LAI includes three tasks.

(1) Determine the effective measurement range: using LAI-2200 instrument needs to pay attention to two angles, one is to avoid direct sunlight and surveyors' shadow, and the other is to prevent LAI-2200 viewing beyond the sample plot range. The former can be covered with masks (e.g., 180 ºC), while the latter needs to be calculated according to the height of the crop. The most wide zenith angle of LAI-2200 is 68°, corresponding to the ground view angle of 22°, with Tan (22°) = 0.404. Since the height of winter wheat is 80 cm, its horizontal distance in LAI-2200 sensor is about 200 cm. In other words, the sensing range of LAI-2200 sensor may exceed the sample plot if it is within 200 cm of the sample plot edge. Therefore, the most reliable measurement area should be within 6 m × 6 m of the center of the sample plot, as shown in Figure 1.

(2) Clean the underlying senescent leaves: when winter wheat upper canopy closed, its leaves in the lower part begin to decline. The LAI measurement accuracy of these withered leaves is usually low. Therefore, it is necessary to clean the senescent leaves near the ground, especially those close to the sensor, to ensure that there is no interference in the field of view

of LAI[15].

(3) Removal of wheat canopy dew: The optimal time for LAI measurement is around sunrise in the morning, but it is often accompanied by dew, so it is necessary to remove the canopy dew gently with a bamboo pole.

3.3.3.2 Leaf Treatment Before SPAD Measurement Wheat leaves may be tarnished by various filths (dust, remnant of foliar fertilization and pesticide, insect excrement, water vapor), if not cleaned in advance, this dirt may contaminate the SPAD lens, resulting in systemic measurement error. These tarnished leaves can be cleaned with clean water and absorbent paper.

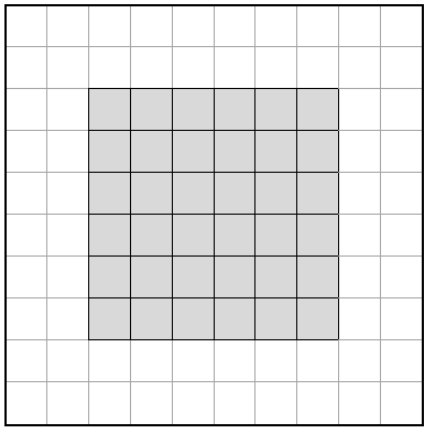

Figure 1 Effective area of sample plot: for a 10 m×10 m plot and 80cm-high winter wheat, the 6 m×6 m section at the center is the effective area and LAI can be measured more accurately

3.3.4 LAI and SPAD Observation

(1) LAI measurement: LAI can be measured within effect area around sunrise and sunset (6–10 a.m., 16–18 p.m.) in sunny days, or the whole day on steady overcast days. Measurement can be conducted along three transects, with an A-BBBBB-BBBBB-BBBBB mode. The average value of the measurement is used to represent the LAI of the sample plot (Figure 1).

(2) SPAD measurement: SPAD-502 is used to measure SPAD along three transects within effect area. Ten leaves from each transect (upper two leaves) are chosen to measure SPAD values, each leaf is evenly measured ten times (avoid main veins), the mean value of all measurements in one plot represents the SPAD value of this plot.

3.4 Retrieval and Processing of Canopy Chlorophyll Content from Sentinel-2

3.4.1 Retrieval of Canopy Chlorophyll Content Products from Sentinel-2

Level 2A acquisition: Level 2A data can be downloaded from the sentinel data website[1]. After checking L2A's quality flags, it is found that the two most recent clear day satellite sensing times with the sampling area are April 29, 2020 and May 19, 2020 respectively (Table 2).

Table 2 Sentinel-2 Level-2A data used to retrieve canopy chlorophyll content

Sensing Date	L2A file name
2020-04-29	S2A_MSIL2A_20200429T025551_N0214_R032_T50SMF_20200429T061414.SAFE
2020-05-19	S2A_MSIL2A_20200519T025551_N0214_R032_T50SMF_20200519T070151.SAFE

(2) Principle of CCC inversion algorithm and development of CCC products: ESA adopts hybrid algorithm for production of CCC products based on Sentinel-2, that is, using PROSAIL model to generate simulation data, and then inputting spectral data into trained artificial neural network (ANN) for inversion.

This algorithm is integrated into the Biophysical processor module of SNAP software. The Sentinel-2 L2A inputs are 8 reflection bands and 4 geometric bands. The output was Canopy Chlorophyll Content, CCC (μg/cm^2). The eight reflection bands are B3, B4, B5, B6, B7, b8a, B11, B12; the four geometric bands are: sun_zenith, sun_azimuth, view_zenith_ mean, view_azimuth_mean.

3.4.2 Temporal Normalization of $CCC_{Sentinel}$ and CCC_{Field}

[1] https://scihub.copernicus.eu/dhus/#/home.

Due to the difference of observation times (Table 3), CCC_{Field} and $CCC_{Sentinel}$ cannot be directly compared. To normalize $CCC_{Sentinel}$ from its satellite date to field observation date, we assume that $CCC_{Sentinel}$ changes linearly during the two satellite observations (20 day interval, Table 2), thus $CCC_{Sentinel}$ can be interpolated to that of field observation date, based on the inverse time interval weight, as expressed in equation (4) and (5).

Table 3 Winter wheat canopy chlorophyll content observation time: field vs. satellite

Month	April		May																		
Date	29	30	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
Sentinel-2	■																				■
Field											■	■	■	■	■	■	■	■			

$$CCC_{Field} = (1-W) - CCC_{0429} + W \times CCC_{0519} \quad (4)$$

$$W = T/\,(T_2-T_1) \quad (5)$$

where, (T_2-T_1) are temporal interval of two Sentinel-2 observations, here is 20 d (from 20200429 to 20200519). T_1 is the temporal interval from first Sentinel-2 observation to field survey.

3.4.3 Field Observation Data Quality and Validation Application

While purpose of field observation is to validate $CCC_{Sentinel}$, field observations are not error free. Using CCC_{Field} to validate the accuracy of $CCC_{Sentinel}$ can also check the quality of CCC_{Field} itself, to some degree. Two forms are used for CCC_{Field}: one uses absolute value, which is calculated by equation (1); and the other is the relative value, which comes from equation (3). R^2 and RMSE were chosen as quality indicator of $CCC_{Sentinel}$.

4 Data Results and Validation

4.1 Data File Organization

The data files are archived into three folders:

(1) Shapefile: field observation data from 107 samples (including LAI; SPAD; CCC_{Field}, Unitless), and corresponding $CCC_{Sentinel}$ (μg/cm^2) developed from Sentinel-2 L2A imagery (interpolated to field observation date).

(2) Excel file: exported from Shapefile, and annotated to serve as a data dictionary.

(3) Tiff file: $CCC_{Sentinel}$ (μg/cm^2) imagery on two dates (20200429, 20200519).

4.2 Data Results

Based on whether SPAD or LCC is used to calculate CCC_{Field}, CCC_{Field} can be expressed in two forms: relative canopy chlorophyll content (CCC_{Field}=LAI × SPAD, Unitless) and absolute canopy chlorophyll content (CCC_{Field} = LAI × LCC, μg/cm^2).

Compared with Sentinel-2 CCC, the ground observation has the following characteristics (Table 4): (1) LCC is larger than SPAD; (2) The average value of “absolute Canopy Chlorophyll” (CCC_{Field}, μg/cm^2)is larger than that of “relative Canopy Chlorophyll”(CCC_{Field}, Unitless), and the range is also larger; (3) The “absolute Canopy Chlorophyll”(CCC_{Field}, μg/cm^2)is slightly larger than the average $CCC_{Sentinel}$ (295.856), but the standard deviation was slightly smaller (98.491).

4.3 Application of Field Sample Data to Sentinel-2 CCC Validation

(1) By absolute value: the coefficient of determination (R^2) of CCC_{Field} and $CCC_{Sentinel}$ of five regression models were calculated, all above 0.889,9 and with an average of 0.9115. The slope of the linear model is 0.989,5, and there is no obvious systematic deviation (Table

5, Figure 2).

Table 4 Chlorophyll Content of winter wheat: field observation and Sentinel-2

	LAI (Unitless)	SPAD (Unitless)	LCC (μg/cm²)	CCC_{Field} (Unitless)	CCC_{Field} (μg/cm²)	$CCC_{Sentinel}$ (μg/cm²)
Min	1.798	44.5	37.698	92.033	82.536	100.435
Max	6.677	64.1	78.313	414.642	490.727	455.677
Average	4.398	58.8	66.076	260.967	295.856	292.667
Std. Deviation	1.219	3.6	7.622	79.360	98.491	101.742

Table 5 Regression analysis of winter wheat Canopy Chlorophyll Content (CCC) from field observation and Sentinel-2 L2A imagery: two methods

Fitting model	Expression of CCC by relative value x= $CCC_{Sentinel}$ (μg/cm²) y= CCC_{Field} (Unitless)	R^2	Expression of CCC by absolute value x= $CCC_{Sentinel}$ (μg/cm²) y= CCC_{Field} (μg/cm²)	R^2
Linear	$y = 0.7525x + 40.721$	0.930,8	$y = 0.9895x - 0.087$	0.917,6
Exponential	$y = 92.648e^{0.0033x}$	0.915,2	$y = 81.103e^{0.0041x}$	0.9
Logarithm	$y = 179.24\ln(x) - 743.05$	0.913,3	$y = 237.54\ln(x) - 1042.3$	0.889,9
Power	$y = 2.5266x^{0.8179}$	0.945,2	$y = 0.9342x^{1.0089}$	0.928
Polynomial	$y = 0.0001x^2 + 0.6982x + 46.862$	0.930,9	$y = -0.0006x^2 + 1.3493x - 43.702$	0.922,1
Average		**0.927,1**		**0.911,5**

(2) By relative value: the relative CCC was calculated using equation (3). All five coefficients of determination (R^2) of ground observation and satellite canopy CCC were above 0.913,3, with an average of 0.927,1, which was significantly higher than that of absolute model. This shows that the correlation with remote sensing is stronger when the ground is only optical observation. However, due to the different units, the slope of the linear model is 0.752,5, which obviously deviates from the 1:1 line and cannot directly explain the quantitative relationships (Table 5).

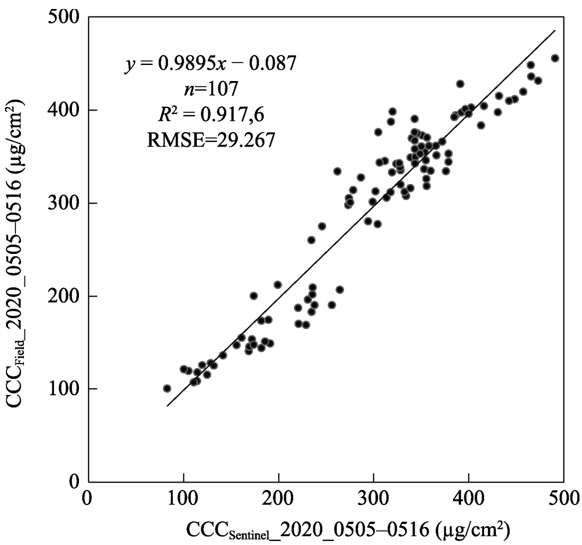

Figure 2 Regression of CCC_{Field} and $CCC_{Sentinel}$ by linear fitting

5 Discussion and Conclusion

(1) To obtain quality ground data, we need to accurately plan the field observation. In this study, the uncertainties in space, time and sampling were minimized as far as possible.

- To minimize spatial uncertainty resulted from small parcels, the effective measurement area is defined based on the sample plot center.
- To temper the temporal uncertainty caused by the date discrepancy of field survey and Sentinel-2 sensing, an inverse time interval weight is used to interpolate original $CCC_{Sentinel}$ to $CCC_{Sentinel}$ corresponding date to field survey.
- In addition, the sample plots and wheat leaves were pretreated to prevent possible systematic deviation in the measurement process of LAI and SPAD.

(2) Possible deficiencies: First, the original LAI measurement is used without further

refinement, and Clumping Index (CI) is not considered. Secondly, SPAD is the result of measuring “clean leaf”; but Sentinel-2 covers actual wheat canopy, clean or otherwise. Third, the SPAD-LCC transformation model is not developed from the same region, but from Luoyang city, Henan province in April 2018.

(3) Conclusion: Although there may be some shortcomings, the analysis results show that, on the whole, the quality of ground observation data and satellite inversion data is very good. The coefficient of determination (R^2) of linear regression between CCC_{Field} and $CCC_{Sentinel}$ is 0.917,6, with a close to 1:1 line and RMSE of 29.267. In comparison, a similar validation conducted by Xie *et al.* (2019)[23] , which is also for winter wheat $CCC_{Sentinel}$ in same season (April–May, 2018) yet different location (Shunyi, Beijing), yields a R^2 of 0.72 and a RMSE of 108.30. Parry *et al*. (2014) [5] suggested that varieties and management have little effect on SPAD-LCC conversion model, which partly explains that the SPAD- LCC model from Luoyang performs quite well in this study. Table 4 shows that the CCC range of ground observation is 82.536–490.727 (μg/cm^2), which indicates that $CCC_{Sentinel}$ can explain the variation of CCC_{Field} value in a wide range, and the validation dataset can be applied to validate winter wheat $CCC_{Sentinel}$ with medium and high coverage.

Author Contribution

Wang, Z. X. designed the dataset development and finished the data paper writing. Li, F. participated in data collection and analysis.

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Conflicts of Interest

The authors declare no conflicts of interest.

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