Paper

A Vector Analysis of Squid Retinal

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Abstract: The chemical substance retinal is easily seen using software for molecule viewing. However it is difficult to understand the three-dimension structure of chemical substances and so we suggest the method of vector analyses. Under that method we exploit the fact that the three-dimensional structure of the chemical substances is such that two straight lines have no crossing point when they are located in parallel in three-dimensional space. Hence we looked at the chemical substance retinal in the light of vector products of each bonding carbon site. In particular we explored if the hexagonal part of retinal is located in a single plane or not. This is quite a difficult question for non-visual methods. To resolve these points we used a vector analysis of the results of the vector products. This is the key point to exploit vector products.

Key words: Structure of squid retinal, Vector analysis, Vector products, Norm distribution of vectors

1. Introduction

In recent times we have been analyzing the structure of squid retinal. Firstly we looked at retinal structure by calculating the charge distributions, and electron orbitals around the chemical substance retinal [1]. We also explored the nearest amino acids around retinal carbon atoms [2]. We also determined what kind atoms are located near every retinal atom [3]. We then calculated dihedral angles to understand the form of the conformation change in squid retinal caused by absorbing light [4]. For this purpose we should utilize vector analyses of retinal bond between every carbon. Here we report on the results of vector analyses for vectors produced by vector products of faced bonds connected to each carbon of retinal. We also determined the direction of the hexagonal part of retinal relative to the zigzag tail carbons. We imaged the vector structure of this bonding part can described by vectors produced by the vector product between the triangle and the faces of the tail bonds. The triangular part should be described by a vector like the sum of two vectors that form the triangle. Thus we conclude that the vector products of required carbon sites represent the retinal structure. We used the set of vector products of each retinal carbon and the resulting description of connection of the hexagonal and the tail parts may be sufficient to provide a mechanical illustration of retinal structure without any assumptions.

We surveyed the literature on vector analysis [5], and curvature [6,7]. We then instantiated a vector analyses for squid retinal. The vector assignments are shown in section 2. It is an important point to understand the structure of squid retinal. The method of vector analyses is applicable for any type of retinal, or other structure that one wants to understand in a concise manner. In section 3 and 4, we present the results for the distribution of vector products across different crystallo-

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graphic data sets. Section 3 is devoted to the vector products between the hexagonal ring of retinal and its tail carbons. Section 4 is restricted to the relationship between the hexagonal and tail parts, in particular how the magnitude of the angles varies between the two parts. For this purpose we utilize the inner product of pairs of vectors. One of these products describes the triangular edged at carbon C_6, and another is corresponds to the tail elements C_6 to C_7 (Fig. 1). The triangle can be described by the vector arising from the vector product between C_6–C_1 and C_5–C_6. If we take the normalized vectors to describe the triangle and tail, i.e. the direction cosines, then the two vectors are orthogonal to each other when inner product is zero when two vectors become close or open to each other when the inner products go to 1 or -1. In section 5, we discuss the obtained results.

2. Retinal carbon numbering and Definition of vectors for carbon string

We illustrate our numbering scheme for the carbons of squid retinal in Fig. 1. The numbering is the same as in our previous papers [1–4]. As mentioned in the Introduction, we can understand the structure of squid retinal in a mechanical manner, in the other words, automatically and free from any model assumptions. A good understanding of the structure of squid retinal can be achieved by the understanding of vector assignments to carbons of squid retinal.

The hexagonal part of retinal is identified by carbon numbers from 1 to 6, and the zigzag tail of retinal encompasses carbons 7 to 15. Main structure of retinal includes both the hexagonal part and the tail. Actual retinal takes a three-dimensional structure.

For a vector analysis of retinal, we must define the vectors using carbon coordinates because of their three-dimensional features. Definition of the vectors for carbons of retinal included is based upon our carbon numbering scheme. That carbon numbering is already shown in Fig. 1 and employed numbers from 1 to 15 producing a set of three numbers for the coordinates of every carbon, namely:
1: C_1–C_2, 2: C_2–C_3, 3: C_3–C_4, 4: C_4–C_5, 5: C_5–C_6, 6: C_1–C_6, 7: C_6–C_7, 8: C_7–C_8. 9: C_8–C_9,
10: C_9–C_{10}, 11: C_{10}–C_{11}, 12: C_{11}–C_{12}, 13: C_{12}–C_{13}, 14: C_{13}–C_{14}. C_{15}: C_{14}–C_{15}.
To know whether each faced-vector is straight or not, we looked at the vector produced by the vector product of each of the faced-vectors. We developed an easy nomenclature using the number 1 to 14. Vector products were shown using numbers 1 to 15. In other words, 1: 1 and 2, 2: 2 and 3, 3: 3 and 4, 4: 4 and 5, 5: 5 and 6, 6: 1 and 6, 7: 7 and 8, 8: 8 and 9, 9: 9 and 10, 10: 10and 11, 11: 11 and 12, 12: 12 and 13, 13: 13 and 14, 14; 14 and 15.

The hexagonal ring is described by vectors from 1 to 6, namely the set of norms obtained from

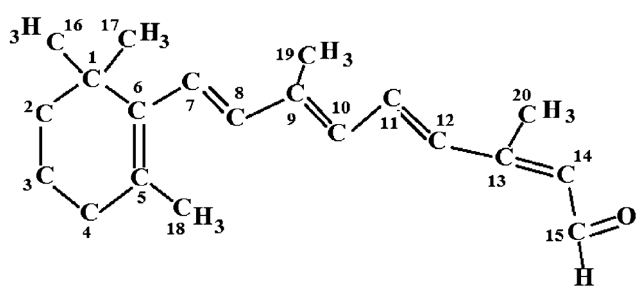

Fig. 1 Numbering of squid retinal carbons

carbons C_1 to C_6. The structure of the tail of retinal can be known from the values of the norm of vector products faced carbons C_6 to C_{15}. We put norm values on the center carbons, each according to its ordinal carbon number. Hence we should consider what quantities to describe the retinal structure. It is known from the structure of retinal that dividing two ways at the carbon C_6 implies two norms exit there. Thus we see whether or not the hexagonal ring cross the tail carbons by the values of the inner products between triangle C_1–C_5–C_6 and tail vector C_6–C_7. The distribution of the norms of vector products is shown in section 3, and the relation of the hexagonal ring to the tail will be described in section 4.

3. Magnitude of the vector generated by the vector product of neared two retinal vectors

We can determine the location of three coordinates from ID codes 2Z73, 2ZIY, 3AYM, and 3AYN of the Protein Data Bank (PDB). To describe the structure of squid retinal, we computed the value of vector products for the faced two vectors for each of the specified carbons. The results are tabulated and list is shown in Table I.

We did not explore the methyl group for carbon number from 16 to 20, since our main interest is concentrated on the configuration relation between the hexagonal ring and tail of retinal. For ease of presentation, we draw the figures of hexagonal part and tail part for PDB identification code 2Z73, 2ZIY, 3AYM, and 3AYN. As seen from Table I, 2ZIY lacks the chain B structure, so we have only chain A information about retinal from PDB id 2ZIY. These results are in the following figures for comparison.

Examining Fig. 2 to Fig. 5, we can see that the same PDB id has the same location in the hexagonal part of squid ring, whereas the tail part for 3AYM has a difference between chain A and

Table I Values of Retinal Vector Products

Numbers 1 to 6 give the values of vector products for hexagonal part of retinal. Number 7 to 14 represent the zig-zag the tail of the retinal molecule. We do not calculate the vector product of carbon line C_6-C_7-C_8.

Center C No	2Z73		2ZIY		3AYM		3AYN	
	Chain A	Chain B	Chain A	Chain B	Chain A	Chain B	Chain A	Chain B
1	2.25381	2.25537	2.22322		2.35577	2.32052	2.29386	2.28514
2	2.13072	2.14022	2.22420		1.99780	1.96951	2.11477	2.11943
3	2.15580	2.16607	2.00594		1.97642	1.94777	2.14343	2.13601
4	2.16744	2.16725	2.01121		2.10341	2.11872	2.11752	2.11703
5	1.76407	1.78595	1.88581		1.78544	1.85323	1.79820	1.79016
6	1.84241	1.84775	1.95842		1.86754	1.90768	1.87068	1.84993
7	1.75701	1.73300	1.74302		1.67599	1.61849	1.61959	1.59655
8	1.53082	1.52336	1.30317		1.51200	1.55741	1.50059	1.51982
9	1.81188	1.80665	1.66570		1.81006	1.77392	1.66809	1.67222
10	1.45554	1.45659	1.53037		1.45009	1.56471	1.54893	1.56375
11	1.56088	1.57910	1.54828		1.75218	1.70154	1.50598	1.53251
12	1.46802	1.48151	1.37170		1.50785	1.67197	1.60329	1.59639
13	1.79395	1.78464	1.66835		1.66440	1.70578	1.70225	1.69303
14	1.67721	1.69821	1.62905		1.64326	1.65736	1.65660	1.65514

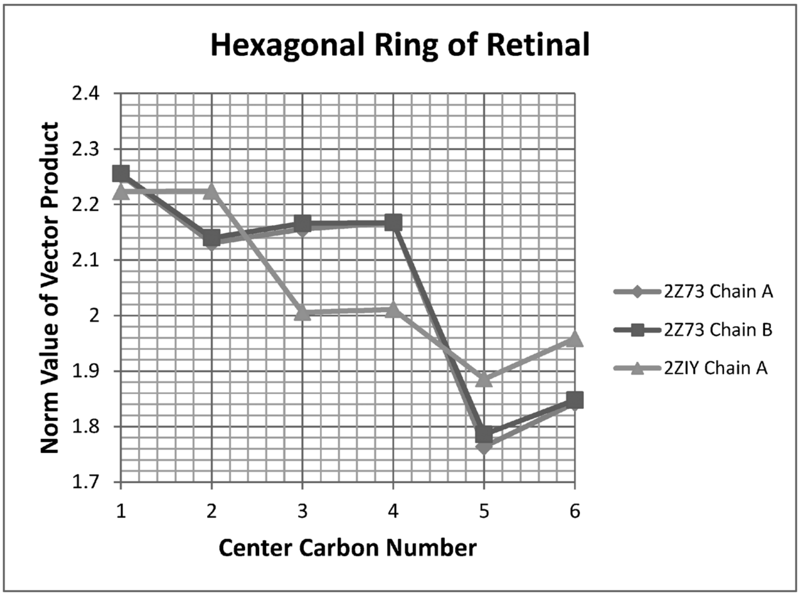

Fig. 2 Hexagonal ring part of the squid retinal for three PDB data
Numbering follows the scheme of Fig. 1

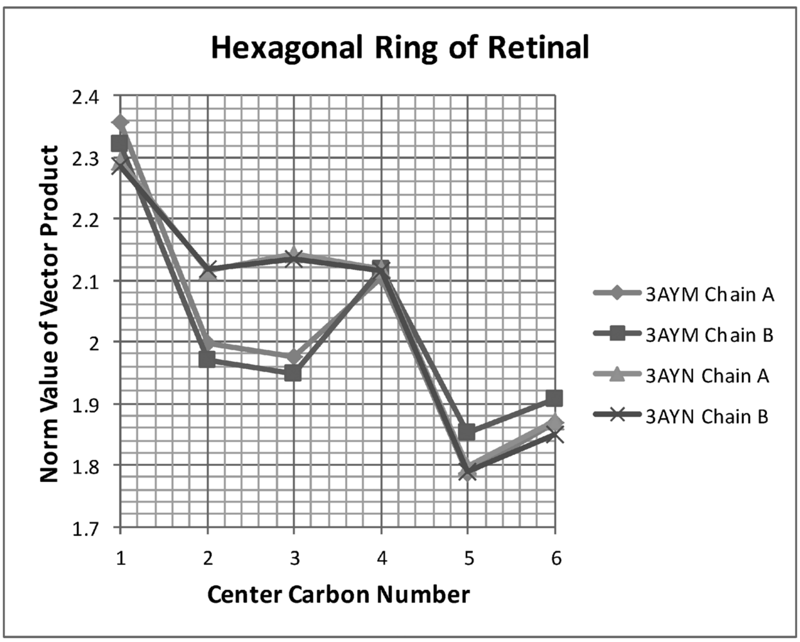

Fig. 3 Hexagonal ring part of the squid retinal for four PDB data
Numbering follows Fig. 1

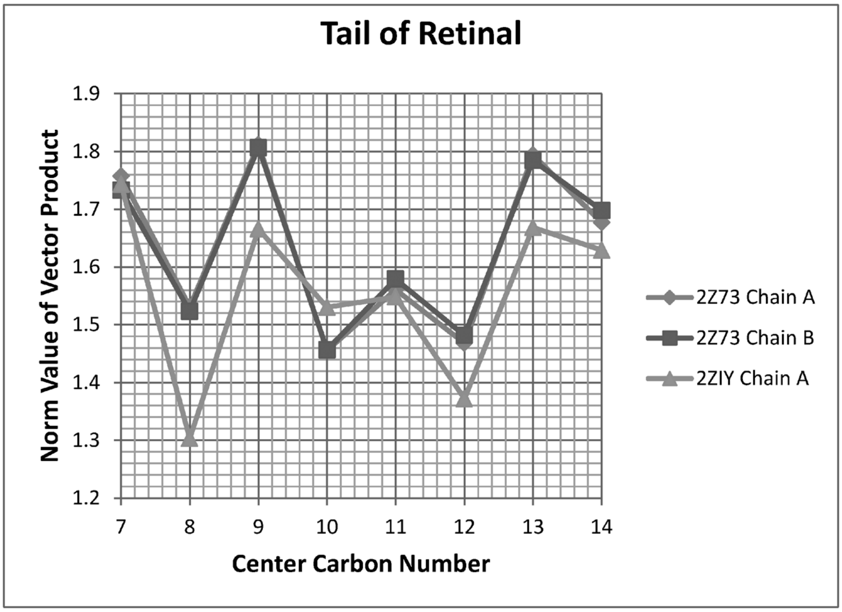

Fig. 4 Tail part of squid retinal for three PDB data
Numbering follows Fig. 1

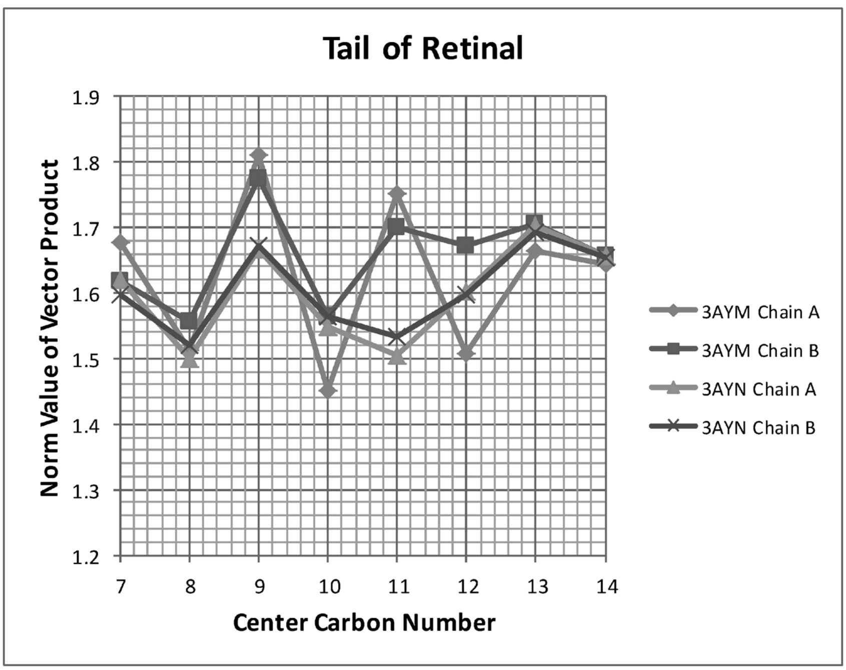

Fig. 5 Tail part of the squid retinal for four PDB data
Numbering follows Fig. 1

chain B. In comparing the ring parts of 3AMY and 3AYN, a difference between chain A and chain B at carbons 2 and 3 is seen in Fig. 3. This difference may be related to a change of structure between chain A and chain B. When comparing Fig. 4 and Fig. 5, the opposite location change can be seen at carbon C_{11}: namely the same position (Fig. 4) while in a different position for 3ANY and 3AYN (Fig. 5). The accepted wisdom is that light absorption by retinal causes a structural conformation change [8]. That transition between the cis-type and trans-type retinal is said to occur between C_{11} and C_{12}. This conformation change may be a rotation of the bond between the nearest carbons.

4. Relationship between the hexagonal and tail parts of squid retinal

We utilized the inner product between the hexagonal ring and the tail of retinal. They connect at the carbon C_6. Hence we know the vectors around carbon C_6 have an important role. The hexagonal ring vector is selected as the triangle C_5–C_6–C_1 only, while the tail vector is the shortest one: C_6–C_7. These vectors and two inner products 1 (vector product of the triangle) and 2 (vector sum of the triangle) are listed in the Table II.

As seen from Table II, inner product 1 takes values near zero, and inner product 2 takes values near one. These results are consistent since inner product 1 used a vector product to denote the triangle while inner product 2 used the vector sum of the two vectors that describe the two carbon bonds C_1–C_6 and C_5–C_6. From inner product 1, the triangle differs a little bit from the tail. The equivalent angles are from -0.6° to 5°. From inner product 2, the triangle has a steep structure. Those angles range in value from 10° to 17°. These two vectors have a different nature: namely the vector product expresses that the triangle is a little bit sloping from the tail vector. But the vector sum to denote the triangle is included in the vectors of the triangle. Thus we conclude that inner product 2 denotes the exact slope of the triangle. We therefore conclude that the triangle to

Table II Inner product between triangle and tail vectors of squid retinal
For the inner product, we used two kinds of vectors. The first was the vector products for carbon line (C_5-C_6-C_1), and the vector sum of two vectors (carbon bond C_5-C_6 and carbon bond C_6-C_1) to denote the hexagonal ring part. Inner products were taken for those vectors and the vector (carbon bond C_6-C_7) to denote tail part of retinal.

		2Z73		2ZIY	3AYM		3AYN	
		Chain A	Chain B	Chain A	Chain A	Chain B	Chain A	Chain B
Vector (C_6-C_7)	X	−0.72517	0.782966	0.467713	−0.74887	0.689105	−0.69858	0.808294
	Y	0.36587	−0.25436	−0.49195	0.269647	−0.39702	0.412381	−0.24595
	Z	−0.58329	0.567683	0.734322	−0.60537	0.606225	−0.58475	0.534948
Vector sum (C_6-C_1) and (C_5-C_6)	X	−0.83256	0.830636	0.412362	−0.89966	0.825482	−0.82199	0.845642
	Y	0.346037	−0.35599	−0.34352	0.271784	−0.43766	0.33341	−0.34421
	Z	−0.43255	0.428155	0.843771	−0.34167	0.356412	−0.46171	0.407931
Vector product of carbons (C_5-C_6-C_1)	X	−0.22199	−0.51013	0.908753	−0.22329	−0.52605	−0.20336	−0.49892
	Y	−0.92386	−0.79472	0.243425	−0.95258	−0.82544	−0.90139	−0.78134
	Z	−0.31179	0.328905	−0.33897	−0.20671	0.204746	−0.38228	0.374974
Inner product for normalized vectors	1	0.004838	−0.01055	0.056367	0.035489	0.089337	−0.00611	−0.01052
	2	0.982657	0.983966	0.981463	0.953859	0.958671	0.981698	0.986407

describe hexagonal ring takes some rotational structure relative to the tail vector and has a little bit of a tilt angle that can be said almost on a plane.

5. Discussion

From vector analyses using vector products, we can quantify the structure of squid retinal. We determined the structural change at the C_{11} carbons by comparing 3AYM and 3AYN. The conformational change is caused by the absorption of light [8,9,10,11]. We also found that no location change occurred at C_{11} from Fig. 4. The fact implies either that no light absorption occurred there or the same state is taken for both crystallizations. We also determined the carbon location change of carbons within the hexagonal ring. This conformation change implies deformation the ring part of squid retinal, but this deformation is slight. We therefore know that a few carbon locations contribute to the deformation of the hexagonal ring part of squid retinal.

Our main interest in this paper: the hexagonal ring part, either takes a direction orthogonal to the tail of squid retinal or not. In the RasMol picture or electron orbital figures, we could not recognize whether the relationship between the hexagonal and tail part of squid retinal is orthogonal to each other or not. For this reason we analyzed the squid retinal from the viewpoint of vector products and inner products. As discussed at section 4, the ring part of squid retinal has a slight tilt relative to the tail part of squid retinal. We conclude that the hexagonal ring may rotate that angles, however we could not estimate the magnitude of the angle from the data since they are embedded in three-dimensional space. In three-dimensional space, it is difficult to determine whether two vectors are parallel or converging. Usually two vectors converge when they are not parallel in the exact sense of the Euclid picture. This scope requires a mechanical picture of the relationship between hexagonal ring and tail carbons of squid retinal. Our point for discussion is taken from sections 4 and 5. We couldn't determine the magnitude of the rotational angle from the PDB data because the tail is a line. The relation between surface and line presents a difficult problem as to how much rotation occurs around the tail line. Our result is that hexagonal ring and tail of squid retinal are located on an almost flat plane from a local perspective.

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