Supporting Information for

Why 11-*cis*-retinal? Why Not 7-*cis*-, 9-*cis*-, or 13-*cis*-Retinal in the Eye?

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I. Computational details.

1. **For the system setup of Bovine and Squid rhodopsins see references 1-7.**

   To evaluate the local environmental perturbations that stabilize or destabilize the retinal in opsin, PSB11 is replaced by PSB7, PSB9 and PSB13 isomers and only the retinal isomer plus residues within 4.0 Å environment of any atom of the retinal isomer are allowed to relax during optimization. The QM model part consists of the **full 7/9/13-*cis*-retinal** (with +1 charge) and side-chain N–H moiety of Lys296(Bovine)/Lys312(Monkey)/Lys305(Squid) along with the hydrogen link atom at the QM/MM boundary. All the calculations are performed using the hybrid QM/MM (QM=B3LYP/6-31G*;MM=AMBER96) protocol in ONIOM (Our own *N*-layer Integrated molecular Orbital plus molecular Mechanics) method with electronic embedding (EE) scheme implemented in Gaussian03.[8]

2. **System setup of Monkey Rhodopsin:** Compared to bovine rhodopsin that contains 348 amino acids, monkey rhodopsin is also composed of the same number of amino acids (AA). However, 22 AA sites are different between bovine and monkey rhodopsin (22/348)[9] and they correspond to K16A, A26Y, M49V, L112A, V173F, M183L, P194L, H195K, E196P, T198V, I213T, L216M, L266V, G270S, D282N, T297S, S298A, A299S, V300I, V318L, L321I and T335A, respectively. Although Glu113 serves as the counterion in both the vertebrate pigments, the large difference in AA sites near the retinal-K296 binding site (T297S, S298A, A299S, V300I) encourages us to include monkey rhodopsin into the investigation.

3. **Residues within 4.0 Å radius of any atom from the retinal in Bovine (Monkey) Rhodopsin:**

   The following residues are relaxed during optimization: Tyr43, Met44, Leu47, Met86, Phe91, Thr94, Glu113, Gly114, Ala117, Thr118, Gly121, Glu122, Leu125, Tyr178, Glu181, Ser186, Cys187, Gly188, Ile189, Tyr191, Met207, Phe208, His211, Phe212, Phe261, Trp265, Tyr268, Ala269, Ala292, Phe293, Phe294, Ala295, Lys296, Thr297 (Ser297 in Monkey), Ser298 (Ala298 in Monkey), Ala299 (Ser299 in Monkey), wat2a, wat2b.

4. **Residues within 4.0 Å radius of any atom from the retinal in Squid Rhodopsin:**

The following residues are relaxed during optimization: Ile41, Phe83, Asn87, Met92, Tyr111, Gly112, Gly115, Gly116, Gly119, Phe120, Ile123, Tyr177, Glu180, Asn185, Cys186, Ser187, Phe188, Met204, Phe205, Phe209, Phe270, Trp274, Tyr277, Ala278, Ala281, Gln298, Val301, Met302, Phe303, Ala304, Lys305, Ala306, Ser307, Ala308, wat502, wat509, wat1, wat2. For wat1 and wat2 positions see reference 4.

II. Energy Decomposition Analysis

LME: Low system model energy – $E^{MM,model}$
HME: High system model energy – $E^{QM,model}$
LRE: Low system real energy – $E^{MM,real}$

$$E^{ONIOM} = E^{MM,real} + E^{QM,model} - E^{MM,model}$$

where $E^{MM,real}$ is the MM energy of the entire system, called real system in ONIOM terminology; $E^{QM,model}$ is the QM energy of a part of real system that has main chemical interest, called model part; $E^{MM,model}$ is the MM energy of the model part.

Stepwise Procedure

STEP 1 = [column **6** of 11-cis] **–** [column **6** of mutant];
HM, nonv = $E^{QM//ME,model}$

STEP 2 = [column **3** – column **5** of 11-cis] - [column **3** – column **5** of mutant];
MM = LR, v - LM, nonv = $E^{MM/EE,\ real} - E^{MM/ME,\ model}$

STEP 3 = **STEP 1 + STEP 2;**
ME = HM, nonv + MM

STEP 4 = **[**column **2** – column **6** of 11-cis**] - [**column **2** – column **6** of mutant**];**
ESP (HM) QM = [$E^{QM//EE}$ – $E^{QM//ME}$ of 11-cis] - [$E^{QM//EE}$ – $E^{QM//ME}$ of mutant];

STEP 5 = **[**column **1** - column **5** of 11-cis**] - [**column **1** - column **5** of mutant**];**
ES (LM) = LM, v – LM, nonv = [$E^{MM/EE,\ model} - E^{MM/ME,\ model}$ of 11-cis] - [$E^{MM/EE,\ model} - E^{MM/ME,\ model}$ of mutant**];**

STEP 6 = **STEP 4 – STEP 5;**
*app.*POL = ESP (HM) QM – ES (LM)

STEP 7 = **STEP 3 + STEP 6;**

EE = ME + *app*.POL

Table S1 & S2: Energy Decomposition Analysis for Bovine Rhodopsin

MODEL	QM/MM-EE (Energy in Hartrees)				QM/MM-ME on EE geometry (Energy in Hartrees)			
	E^{MM},model	E^{QM},model	E^{MM},real	E^{ONIOM}	E^{MM},model	E^{QM},model	E^{MM},real	E^{ONIOM}
7-cis	-0.006827	-834.839008	-15.980397	-850.812577	0.151251	-834.678627	-15.980397	-850.810275
9-cis	-0.037027	-834.850517	-16.014405	-850.827895	0.120677	-834.692026	-16.014405	-850.827109
11-cis	-0.034858	-834.847066	-16.017523	-850.829731	0.127053	-834.687077	-16.017520	-850.831651
13-cis	-0.012063	-834.830788	-15.965715	-850.784440	0.134378	-834.682112	-15.965715	-850.782205
Notation	1	2	3	4	5	6	7	8

MODEL	ENERGY DECOMPOSITION ANALYSIS FOR BOVINE (in kcal.mol^{-1})						
	HM.nonv QM part S1	LR,v – LM, nonv MM contribution S2	ME S3 = S1+S2	ESP (HM) QM S4	ES (LM) LM, v – LM, nonv S5	*app*.POL S6 = S4 – S5	EE = ME + *app*.POL S7 = S3 + S6
7-cis	5.302	8.112	13.414	-0.245	2.405	-2.650	10.764
9-cis	-3.105	5.957	2.852	0.940	2.640	-1.700	1.152
11-cis	0.000	0.000	0.000	0.000	0.000	0.000	0.000
13-cis	3.115	27.913	31.028	7.099	9.707	-2.608	28.420

Table S3 & S4: Energy Decomposition Analysis for Monkey Rhodopsin

MODEL	QM/MM-EE (Energy in Hartrees)				QM/MM-ME on EE geometry (Energy in Hartrees)			
	E^{MM},model	E^{QM},model	E^{MM},real	E^{ONIOM}	E^{MM},model	E^{QM},model	E^{MM},real	E^{ONIOM}
7-cis	0.040947	-834.789993	-16.050370	-850.881311	0.149393	-834.679556	-16.050370	-850.879319
9-cis	0.012063	-834.801067	-16.084544	-850.897674	0.119825	-834.692847	-16.084543	-850.897215
11-cis	0.014700	-834.798344	-16.085987	-850.899031	0.126194	-834.688143	-16.085988	-850.900325
13-cis	0.049212	-834.773567	-16.020025	-850.842804	0.146082	-834.674021	-16.020025	-850.840129
Notation	1	2	3	4	5	6	7	8

MODEL	ENERGY DECOMPOSITION ANALYSIS (in kcal.mol^{-1})						
	HM.nonv QM part S1	LR,v – LM, nonv MM contribution S2	ME S3 = S1+S2	ESP (HM) QM S4	ES (LM) LM, v – LM, nonv S5	*app*.POL S6 = S4 – S5	EE = ME + *app*.POL S7 = S3 + S6
7-cis	5.388	7.792	13.18	0.148	1.912	-1.764	11.416
9-cis	-2.952	4.902	1.95	1.243	2.342	-1.099	0.851
11-cis	0.000	0.000	0.000	0.000	0.000	0.000	0.000
13-cis	8.862	28.911	37.773	6.686	9.177	-2.491	35.282

Table S5 & S6: Energy Decomposition Analysis for Squid Rhodopsin

MODEL	QM/MM-EE (Energy in Hartrees)				QM/MM-ME on EE geometry (Energy in Hartrees)			
	E^{MM},model	E^{QM},model	E^{MM},real	E^{ONIOM}	E^{MM},model	E^{QM},model	E^{MM},real	E^{ONIOM}
7-cis	0.061610	-834.776625	-17.885062	-852.723297	0.173526	-834.669706	-17.885062	-852.728295
9-cis	0.021982	-834.789817	-17.927588	-852.739387	0.131275	-834.687911	-17.927591	-852.746777
11-cis	0.027603	-834.786385	-17.928735	-852.742723	0.134737	-834.684103	-17.928735	-852.747575
13-cis	0.039552	-834.772667	-17.905193	-852.717411	0.131540	-834.686097	-17.905193	-852.722831
Notation	1	2	3	4	5	6	7	8

MODEL	ENERGY DECOMPOSITION ANALYSIS FOR SQUID RHODOPSIN (in kcal.mol^{-1})						
	HM.nonv QM part S1	LR,v – LM, nonv MM contribution S2	ME S3 = S1+S2	ESP (HM) QM S4	ES (LM) LM, v – LM, nonv S5	*app*.POL S6 = S4 – S5	EE = ME + *app*.POL S7 = S3 + S6
7-cis	+9.034	3.065	12.099	-2.910	-3.000	0.090	9.099
9-cis	-2.389	2.892	0.503	0.236	-1.355	1.591	2.094
11-cis	0.000	0.000	0.000	0.000	0.000	0.000	0.000
13-cis	-1.251	16.779	15.528	9.859	9.504	0.355	15.883

III. Electronic Spectra Calculations in the Gas phase and Protein environments

All single point *ab initio* QM/MM calculations on the resulting coordinates were carried out with the ORCA 2.6.19 program package[10] using an electronic embedding scheme.[11] We applied three-root spectroscopy oriented configuration interaction (SORCI) method with Davidson correction (+Q) for excitations higher than doubles on complete active space self-consistent field (CASSCF) wave functions to calculate absorption and circular dichroism (CD) spectra. We employed the 6-31G* basis set in all calculations. In multireference *ab initio* calculations, an auxiliary basis set (SV/C) was also used. The active space encompasses 6 electrons in 6 orbitals. Computational efficiency of SORCI+Q calculations was enhanced by setting T_{pre}, T_{nat} and T_{sel} thresholds to 10^{-4}, 10^{-6} and 10^{-6} *E*h, respectively. In the following we abbreviate the ground, first excited singlet states as S_0, S_1.

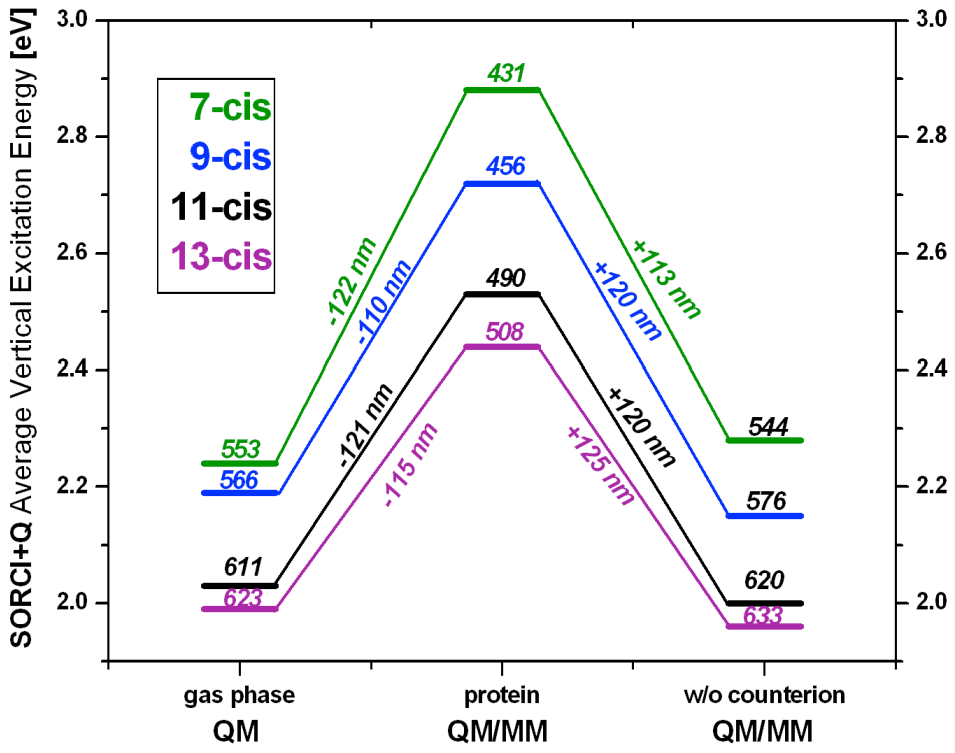

Figure S1 Average values of the SORCI+Q calculated first vertical excitation energies ($S_0 \rightarrow S_1$) between gas phase and protein environments (QM/MM) with and without charges of the counterion (w/o counterion), for PSB7, PSB9, PSB11 and PSB13 retinal isomers in bovine, monkey and squid rhodopsins are plotted.

IV. Distance of SBN^+ to the side chain oxygen atom of E113, E181 residues in bovine, and N87, Y111, E180 residues in squid rhodopsin.

Comparison of difference in distances between the PSB nitrogen atom and side chain oxygen atom of E113 (OE2) and E181 (OE2) in bovine and monkey with N87 (OD1), Y111 (OH) and E180 (OE2) in squid rhodopsins for all the QM/MM optimized geometries.

PSBR	Bovine (Å)		Monkey (Å)		Squid (Å)		
	E113	E181	E113	E181	N87	Y111	E180
PSB7	2.73	6.51	2.72	6.43	2.87	3.31	4.73
PSB9	2.74	6.56	2.73	6.52	3.91	3.29	4.35
PSB11	2.73	6.50	2.73	6.44	3.93	3.41	4.29
PSB13	2.73	6.35	2.73	6.35	3.98	3.51	4.23

V. Average bond lengths along the carbon atoms of the retinal conjugation

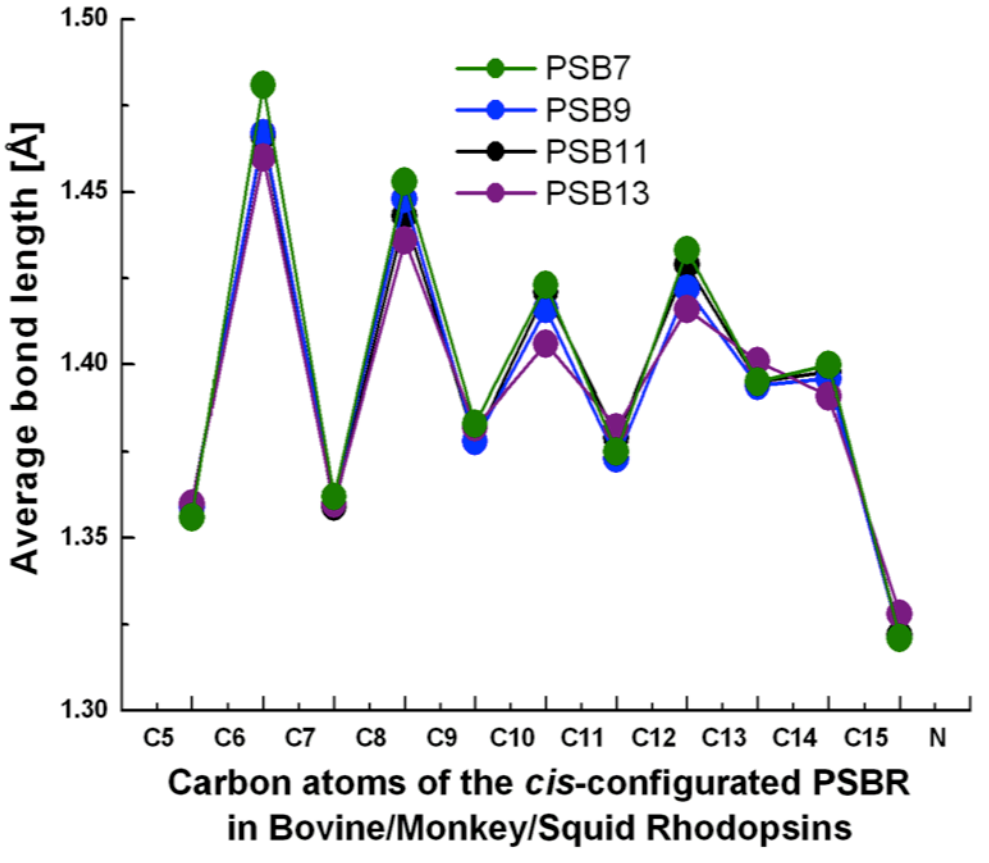

Figure S2 Comparison of average bond lengths along the carbon atoms of the retinal conjugation in vertebrate (bovine, monkey) and invertebrate (squid) visual pigments.

The peaks in Figure S2 correspond to the single-bond lengths, which reach values as long as 1.48 Å for the C6–C7 bond, and the troughs indicate the sharp reduction in the double-bond lengths, which reach values as low as 1.32 Å for the C15=N bond. The average bond-length alternation (BLA) of the C5–N moiety (defined as the average of the lengths of the single bonds minus that of the double bonds) shows a gradual decrease going from PSB7 to PSB13. This decrease is attributed to the increase in localization of positive charge by the counterion at the Schiff base N terminal.[12] The smallest bond angles found at both C9 and C13 are due to the presence of spacious methyl groups, which serves as the signature motif of PSB11. The negative pretwist of the isomerizing double bond is also a characteristic feature of all of the protein-bound retinal isomers.[13] The orientation of the β-ionone ring (C6–C7 dihedral angle) relative to the polyene chain varies from 60° in PSB7 to 40° in PSB13 and was calculated to be different for each isomer.[14] Significant nonplanar distortions (in the range of 10 ± 10°) induced into the chromophore are also a common feature of the retinal chromophore across different visual pigments.

VI. Geometric Parameters of the Retinal Isomers.

PSB7

Bonds	Bovine	Monkey	Squid	Average
C5=C6	1.355	1.355	1.358	1.356
C6-C7	1.482	1.482	1.479	1.481
C7=C8	1.362	1.363	1.362	1.362
C8-C9	1.454	1.454	1.451	1.453
C9=C10	1.382	1.383	1.385	1.383
C10-C11	1.423	1.424	1.421	1.423
C11=C12	1.376	1.375	1.374	1.375
C12-C13	1.432	1.433	1.434	1.433
C13=C14	1.397	1.396	1.393	1.395
C14-C15	1.400	1.402	1.397	1.400
C15=N	1.319	1.318	1.326	1.321

PSB9

Bonds	Bovine	Monkey	Squid	Average
C5=C6	1.359	1.359	1.36	1.359

C6-C7	1.466	1.465	1.471	1.467
C7=C8	1.363	1.364	1.358	1.362
C8-C9	1.447	1.447	1.451	1.448
C9=C10	1.378	1.378	1.377	1.378
C10-C11	1.415	1.415	1.417	1.416
C11=C12	1.375	1.374	1.371	1.373
C12-C13	1.421	1.422	1.424	1.422
C13=C14	1.397	1.395	1.39	1.394
C14-C15	1.395	1.397	1.395	1.396
C15=N	1.321	1.319	1.324	1.321

PSB11

Bonds	Bovine	Monkey	Squid	Average
C5=C6	1.359	1.359	1.361	1.360
C6-C7	1.464	1.465	1.469	1.466
C7=C8	1.36	1.361	1.357	1.359
C8-C9	1.441	1.443	1.444	1.443
C9=C10	1.379	1.378	1.377	1.378
C10-C11	1.42	1.422	1.421	1.421
C11=C12	1.379	1.378	1.379	1.379
C12-C13	1.427	1.43	1.431	1.429
C13=C14	1.397	1.396	1.391	1.395
C14-C15	1.397	1.4	1.397	1.398
C15=N	1.322	1.321	1.324	1.322

PSB13

Bonds	Bovine	Monkey	Squid	Average
C5=C6	1.36	1.36	1.36	1.36
C6-C7	1.456	1.453	1.471	1.46
C7=C8	1.362	1.362	1.356	1.36
C8-C9	1.434	1.432	1.441	1.436
C9=C10	1.384	1.385	1.378	1.382
C10-C11	1.405	1.404	1.41	1.406
C11=C12	1.382	1.383	1.382	1.382
C12-C13	1.417	1.419	1.411	1.416
C13=C14	1.406	1.404	1.394	1.401
C14-C15	1.394	1.393	1.386	1.391
C15=N^+	1.327	1.325	1.331	1.328

PSB7

Bonds	Bovine	Monkey	Squid	Average
C5=C6-C7	119.905	120.147	120.661	120.238
C6-C7=C8	128.721	129.190	128.905	128.939
C7=C8-C9	128.854	129.118	127.788	128.587
C8-C9=C10	119.608	119.458	121.166	120.077
C9=C10-C11	122.234	122.392	120.192	121.606
C10-C11=C12	130.321	130.362	134.406	131.696
C11=C12-C13	120.986	121.234	119.501	120.574
C12-C13=C14	120.531	120.481	120.423	120.478
C13=C14-C15	120.273	120.112	120.619	120.335
C14-C15=N	127.330	127.083	125.693	126.702

PSB9

Bonds	Bovine	Monkey	Squid	Average
C5=C6-C7	121.622	121.496	121.816	121.645
C6-C7=C8	126.562	126.618	124.452	125.877
C7=C8-C9	124.319	124.485	126.266	125.023
C8-C9=C10	124.523	124.799	122.159	123.827
C9=C10-C11	127.657	127.819	122.990	126.155
C10-C11=C12	122.565	122.554	126.716	123.945
C11=C12-C13	125.002	125.200	123.084	124.429
C12-C13=C14	118.547	118.458	119.183	118.729
C13=C14-C15	121.348	121.080	121.281	121.236
C14-C15=N	126.186	125.927	124.200	125.438

PSB11

Bonds	Bovine	Monkey	Squid	Average
C5=C6-C7	121.414	121.340	121.748	121.501
C6-C7=C8	122.993	123.836	122.567	123.132
C7=C8-C9	128.963	128.732	127.903	128.199
C8-C9=C10	117.321	117.798	115.826	116.982
C9=C10-C11	124.841	124.841	128.475	126.052
C10-C11=C12	129.805	130.033	126.459	128.766
C11=C12-C13	130.566	130.716	129.361	130.214
C12-C13=C14	116.756	116.747	117.101	116.868
C13=C14-C15	123.719	123.563	123.500	123.594
C14-C15=N	124.011	123.864	123.102	123.659

PSB13

Bonds	Bovine	Monkey	Squid	Average
C5=C6-C7	122.741	123.065	120.682	122.163
C6-C7=C8	124.266	124.868	119.725	122.953
C7=C8-C9	124.966	124.252	129.846	126.355
C8-C9=C10	116.821	116.429	114.396	115.882
C9=C10-C11	123.324	122.108	131.124	125.519
C10-C11=C12	127.389	129.510	120.290	125.730
C11=C12-C13	120.110	118.765	125.644	121.506
C12-C13=C14	125.924	126.716	125.216	125.952
C13=C14-C15	125.457	125.726	131.220	127.468
C14-C15=N	124.051	124.340	119.968	122.786

PSB7

Dihedral	Bovine	Monkey	Squid	Average
C5=C6-C7=C8	-57.923	-57.570	-57.965	-57.819
C6-C7=C8-C9	-11.916	-11.801	-13.680	-12.466
C7=C8-C9=C10	168.060	170.436	169.978	169.491
C8-C9=C10-C11	176.295	175.996	171.487	174.758
C9=C10-C11=C12	170.590	170.702	175.984	172.425
C10-C11=C12-C13	-177.675	-177.428	176.175	177.092
C11=C12-C13=C14	165.981	166.435	163.134	165.183
C12-C13=C14-C15	-173.828	-173.148	-175.860	-174.279
C13=C14-C15=N	171.678	172.707	161.489	168.626
C14-C15=N-C	175.694	177.409	-174.797	175.967

PSB9

Dihedral	Bovine	Monkey	Squid	Average
C5=C6-C7=C8	-47.985	-47.653	-50.487	-48.708
C6-C7=C8-C9	171.347	171.499	177.168	173.338
C7=C8-C9=C10	174.846	174.807	162.237	170.63
C8-C9=C10-C11	-14.443	-14.109	-17.408	-15.320
C9=C10-C11=C12	176.694	177.390	179.224	177.769
C10-C11=C12-C13	175.909	176.148	169.828	173.962
C11=C12-C13=C14	169.348	169.691	165.703	168.247
C12-C13=C14-C15	-178.514	-177.547	-179.684	-178.582
C13=C14-C15=N	171.553	172.132	162.844	168.843
C14-C15=N-C	176.804	178.999	-176.215	177.339

PSB11

Dihedral	Bovine	Monkey	Squid	Average
C5=C6-C7=C8	-45.472	-44.923	-45.469	-45.288
C6-C7=C8-C9	177.409	176.965	-173.510	175.961
C7=C8-C9=C10	175.897	175.335	160.062	170.431
C8-C9=C10-C11	170.567	171.191	178.902	173.553
C9=C10-C11=C12	173.596	173.012	168.890	171.833
C10-C11=C12-C13	-18.646	-17.195	-17.256	-17.699
C11=C12-C13=C14	174.239	173.674	165.773	171.229
C12-C13=C14-C15	179.451	-179.553	176.110	178.371
C13=C14-C15=N	172.405	172.620	163.167	169.397
C14-C15=N-C	174.213	176.378	179.553	176.715

PSB13

Dihedral	Bovine	Monkey	Squid	Average
C5=C6-C7=C8	-37.704	-35.626	-50.132	-41.154
C6-C7=C8-C9	-162.412	-158.051	-177.428	-165.964
C7=C8-C9=C10	166.310	163.750	165.687	165.249
C8-C9=C10-C11	-159.871	-155.077	174.750	163.233
C9=C10-C11=C12	168.959	165.694	175.512	170.055
C10-C11=C12-C13	178.735	-178.902	172.365	176.667
C11=C12-C13=C14	-165.348	-161.949	176.981	168.093
C12-C13=C14-C15	-25.947	-30.743	-5.655	-20.781
C13=C14-C15=N	171.763	172.125	168.910	170.933
C14-C15=N-C	155.603	156.280	173.684	161.856

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IX. ONIOM (QM:MM) where QM=B3LYP/6-31G*; MM=AMBER96; optimized Cartesian coordinates (in Å) of all the retinal models discussed in this study.

Model 1: Bovine PSB11

51 Atoms

N	45.694430	12.502870	16.364385
H	45.807918	13.373397	16.914726
H	46.444345	12.305347	15.688714
C	35.568625	7.669884	17.142234
C	34.995010	6.241890	17.288725
C	33.702505	6.321771	18.128443
H	32.952901	6.975493	17.676432
H	33.929950	6.733959	19.112773
H	33.266081	5.325390	18.272255
C	35.970925	5.283604	18.004033
H	36.198759	5.598337	19.027142
H	36.916052	5.188017	17.461361
H	35.523240	4.284771	18.068614
C	35.223538	8.465664	16.095637
C	35.575557	9.928031	15.962908
H	36.372887	10.073718	15.222171
H	35.894625	10.387829	16.898835
H	34.692141	10.470690	15.602100
C	34.716811	5.663125	15.885088
H	34.261306	4.670450	15.988319
H	35.678087	5.520899	15.369712
C	33.821342	6.567984	15.042812
H	32.824641	6.620010	15.492403
H	33.692457	6.135658	14.042543
C	34.397880	7.983650	14.926069
H	35.031968	8.065493	14.028753
H	33.585097	8.708361	14.775229
C	36.432612	8.157183	18.218899
H	36.147971	7.894226	19.236736
C	37.574754	8.860050	17.991401
H	37.851853	9.007029	16.952494
C	38.486832	9.440215	18.944544
C	38.191727	9.389086	20.419274
H	37.438774	8.633720	20.641006
H	37.808565	10.345121	20.785965
H	39.092373	9.147788	20.990478
C	39.627532	10.034788	18.447995
H	39.795602	9.960811	17.379603
C	40.533658	10.815884	19.212458
H	40.175547	11.114086	20.194388
C	41.752051	11.354073	18.857318
H	42.133455	12.116700	19.526857
C	42.634430	11.026008	17.784490
C	42.379761	9.826035	16.903419
H	41.716662	10.084853	16.067383
H	41.901359	9.025744	17.471605
H	43.297345	9.421118	16.472648
C	43.752532	11.847084	17.616102
H	43.894133	12.691885	18.287052

C	44.715035	11.652702	16.622000
H	44.680531	10.768083	15.991591

Model 2: Bovine PSB7

51 Atoms

N	45.783636	12.795350	16.569974
H	45.777225	13.702244	17.072340
H	46.588368	12.640353	15.946105
C	35.538834	8.037883	17.609812
C	35.025730	6.578463	17.510573
C	33.940392	6.317654	18.570884
H	33.499796	5.326625	18.413274
H	33.137274	7.060278	18.527464
H	34.377837	6.317797	19.568889
C	36.172808	5.570327	17.772681
H	36.908575	5.564062	16.960341
H	35.763247	4.556508	17.856829
H	36.695107	5.793632	18.709802
C	35.527523	8.889822	16.555598
C	35.850228	10.359091	16.645002
H	36.833194	10.591605	16.210518
H	35.828629	10.746408	17.662848
H	35.115187	10.918382	16.058771
C	34.412342	6.299130	16.120355
H	33.392009	6.705522	16.090149
H	34.331213	5.213153	15.991080
C	35.223738	6.933348	14.996333
H	36.269143	6.606367	15.056663
H	34.858475	6.620286	14.012207
C	35.174002	8.449399	15.151545
H	35.866171	8.933242	14.446868
H	34.170831	8.831340	14.898727
C	35.965730	8.519919	18.944985
H	35.216668	8.453798	19.733715
C	37.150303	9.086927	19.307677
H	37.200882	9.528736	20.300511
C	38.392923	9.162782	18.556839
C	38.547423	8.304339	17.328611
H	38.121615	8.802759	16.457625
H	38.009248	7.366992	17.443957
H	39.586764	8.060975	17.110978
C	39.406746	9.993416	18.996226
H	39.222076	10.634218	19.854476
C	40.672778	10.053261	18.349610
H	40.815953	9.307232	17.581157
C	41.723293	10.923158	18.528318
H	41.657558	11.743878	19.238815
C	42.903411	10.828867	17.723144
C	43.101107	9.608686	16.839592
H	42.709200	9.774716	15.828313
H	42.611566	8.728622	17.252364
H	44.154453	9.352588	16.740143
C	43.832433	11.871825	17.700909
H	43.710293	12.736518	18.348511
C	44.917117	11.832112	16.816565
H	45.067371	10.931767	16.229458

Model 3: Bovine PSB9

51 Atoms

N	45.856494	12.473561	16.177580
H	45.923508	13.310617	16.785749
H	46.598531	12.363689	15.474578
C	35.795100	7.774502	17.161698
C	35.150008	6.373110	17.280538
C	33.856562	6.505020	18.115667
H	33.121467	7.159027	17.641228
H	34.082931	6.941858	19.089805
H	33.396714	5.523184	18.283779
C	36.075770	5.356414	17.980258
H	36.324712	5.651236	19.004259
H	37.012494	5.214813	17.432519
H	35.576497	4.382102	18.039533
C	35.469139	8.608684	16.140145
C	35.860920	10.062166	16.053213
H	34.966825	10.652454	15.810857
H	36.586544	10.222399	15.246987
H	36.283862	10.459576	16.975316
C	34.839217	5.834718	15.867587
H	35.789399	5.662841	15.340848
H	34.342333	4.860200	15.954127
C	33.973134	6.793481	15.053510
H	33.826083	6.394117	14.042001
H	32.979049	6.863176	15.508043
C	34.599581	8.192578	14.973489
H	35.212980	8.282853	14.064564
H	33.810348	8.950218	14.861519
C	36.622372	8.222607	18.285396
H	36.244726	7.966041	19.274746
C	37.798034	8.907337	18.205694
H	38.224439	9.078286	17.221768
C	38.486040	9.482159	19.341599
C	37.803254	9.471558	20.674856
H	37.903186	8.488947	21.148771
H	36.735980	9.679147	20.586177
H	38.240040	10.212212	21.342144
C	39.722932	10.086435	19.281478
H	40.039212	10.639438	20.162019
C	40.665007	10.023857	18.228168
H	40.451146	9.362154	17.395769
C	41.847697	10.725539	18.250246
H	42.021337	11.415064	19.073185
C	42.865447	10.638252	17.263072
C	42.769614	9.577660	16.187072
H	42.292560	9.970223	15.280106
H	42.196471	8.714373	16.527159
H	43.751964	9.206255	15.898382
C	43.906622	11.568665	17.293745
H	43.934532	12.330002	18.070661
C	44.920206	11.555612	16.334979
H	44.953647	10.733438	15.625769

Model 4: Bovine PSB13

N	45.869686	12.475760	16.603118
H	46.335871	13.062553	17.320079
H	46.376103	12.374372	15.714312
C	35.473272	7.905725	16.880619
C	35.082147	6.456492	17.261120
C	34.190604	6.506193	18.520748
H	33.840789	5.496798	18.768515
H	33.315558	7.144181	18.362783
H	34.732703	6.887757	19.388106
C	36.331439	5.597144	17.557591
H	36.954206	5.479261	16.664023
H	36.029629	4.598945	17.895271

H	36.953342	6.031761	18.346559
C	35.053845	8.504998	15.733798
C	35.117154	9.988613	15.467757
H	35.822792	10.227736	14.659354
H	35.384274	10.565241	16.354929
H	34.129313	10.336946	15.135730
C	34.264888	5.792192	16.135251
H	33.227800	6.119640	16.231449
H	34.270639	4.704812	16.267655
C	34.737242	6.209166	14.750542
H	35.812159	6.017855	14.644512
H	34.229178	5.637411	13.965407
C	34.457599	7.702090	14.604364
H	34.865659	8.095422	13.663692
H	33.367408	7.868320	14.561998
C	36.343021	8.567606	17.842388
H	36.262153	8.243908	18.876017
C	37.369001	9.397787	17.504402
H	37.501833	9.662256	16.459047
C	38.444611	9.772363	18.376167
C	38.416984	9.349381	19.822841
H	38.735695	8.306120	19.925101
H	37.403816	9.413837	20.225439
H	39.055197	9.965957	20.454090
C	39.541702	10.378958	17.789383
H	39.442187	10.713474	16.762926
C	40.809108	10.433583	18.394258
H	40.847067	10.108366	19.425224
C	42.001010	10.821949	17.811899
H	41.997462	11.214737	16.796380
C	43.192579	10.844017	18.578183
C	43.172573	10.199888	19.934204
H	42.564343	9.296512	19.940162
H	42.788599	10.901994	20.682038
H	44.179277	9.913275	20.223789
C	44.394300	11.477811	18.216491
H	45.077082	11.753271	19.022742
C	44.809588	11.739675	16.911856
H	44.299676	11.256302	16.078262

Model 5: Monkey PSB11

N	45.715553	12.531986	16.405607
H	45.806286	13.404913	16.956831
H	46.468919	12.354346	15.728037
C	35.567072	7.656151	17.135285
C	34.979680	6.234181	17.288952
C	33.706346	6.329695	18.155347
H	32.937150	6.955461	17.697311
H	33.953300	6.783252	19.116605
H	33.283509	5.335324	18.346889
C	35.964935	5.269146	17.982457
H	36.208457	5.576906	19.004501
H	36.901990	5.179763	17.423799
H	35.518634	4.269488	18.046227
C	35.224320	8.453188	16.088269
C	35.591982	9.910323	15.951689
H	36.393305	10.041688	15.213062
H	35.913135	10.372141	16.885857
H	34.715602	10.459138	15.585322
C	34.662005	5.656500	15.892802
H	34.183233	4.675637	16.006653
H	35.609468	5.486403	15.360513
C	33.775162	6.579782	15.061820
H	32.788241	6.665331	15.527239
H	33.615729	6.143356	14.069524
C	34.391355	7.975258	14.923056
H	35.034042	8.022638	14.029047
H	33.599848	8.718684	14.753594
C	36.436768	8.139962	18.208690
H	36.156122	7.874234	19.227347
C	37.578431	8.845494	17.981263
H	37.852845	8.994326	16.942672
C	38.489885	9.429943	18.932039
C	38.186684	9.391827	20.406375
H	37.459347	8.613284	20.635091
H	37.764828	10.338636	20.753806
H	39.090993	9.194159	20.988775
C	39.633879	10.020803	18.436598
H	39.807412	9.936683	17.369866
C	40.535258	10.812424	19.196846
H	40.170900	11.120415	20.173778
C	41.754092	11.353125	18.846110
H	42.126926	12.120623	19.515340
C	42.647475	11.029000	17.779714
C	42.405969	9.829669	16.894183
H	41.738647	10.083876	16.060282
H	41.936154	9.021751	17.459284
H	43.326314	9.437291	16.457944
C	43.761818	11.856714	17.624146
H	43.889138	12.703208	18.296178
C	44.741094	11.671120	16.642951
H	44.725183	10.787825	16.009552

Model 6: Monkey PSB7

N	45.661812	12.554624	16.473402
H	45.748559	13.354009	17.128103
H	46.390364	12.504787	15.747136
C	35.362819	7.816662	17.675775
C	34.808207	6.382530	17.481909
C	33.837309	6.027359	18.621885
H	33.381413	5.049333	18.429906
H	33.035981	6.766349	18.721941
H	34.372402	5.952317	19.567006
C	35.957669	5.344956	17.511770
H	36.613868	5.432339	16.638121
H	35.544312	4.329098	17.515787
H	36.570201	5.455084	18.413830
C	35.270768	8.767673	16.714532
C	35.630076	10.216963	16.915455
H	36.540212	10.491219	16.363678
H	35.771778	10.492892	17.959663
H	34.821063	10.830861	16.509643
C	34.035521	6.255432	16.149715
H	33.029531	6.677958	16.279549
H	33.908295	5.189717	15.923620
C	34.727685	6.984719	15.003534
H	35.754737	6.615484	14.886733
H	34.220413	6.794938	14.050648
C	34.761619	8.477331	15.318619
H	35.393379	9.012225	14.594393
H	33.754067	8.913305	15.214592
C	35.918119	8.155676	19.007707
H	35.242039	8.005962	19.849829
C	37.137262	8.676780	19.325657
H	37.275268	9.007849	20.353185
C	38.315031	8.832457	18.487773
C	38.339246	8.161489	17.139874
H	37.869540	8.795439	16.387343
H	37.776122	7.231563	17.157108
H	39.348406	7.931379	16.802311
C	39.388956	9.568453	18.954077
H	39.292581	10.086152	19.905325
C	40.604185	9.691689	18.222642
H	40.664138	9.058630	17.349683

C	41.694886	10.501560	18.437582
H	41.710957	11.211387	19.261660
C	42.807738	10.504500	17.534571
C	42.907873	9.430329	16.464492
H	42.530028	9.781163	15.496236
H	42.361302	8.529644	16.735850
H	43.942645	9.124452	16.315573
C	43.769056	11.514940	17.598655
H	43.735467	12.265969	18.384035
C	44.773672	11.592689	16.624122
H	44.827469	10.807020	15.876742

Model 7: Monkey PSB9

N	45.855084	12.579432	16.404608
H	45.902795	13.415565	17.016014
H	46.582129	12.510795	15.681464
C	35.994711	7.437351	17.482312
C	35.421022	6.012533	17.671365
C	34.146546	6.105446	18.542329
H	33.351307	6.669033	18.049709
H	34.357343	6.617230	19.483832
H	33.767666	5.103968	18.781497
C	36.424579	5.072161	18.371888
H	36.679799	5.409710	19.381463
H	37.354942	4.974288	17.802626
H	35.988912	4.070804	18.470380
C	35.646970	8.202015	16.413815
C	35.973369	9.664918	16.260636
H	35.054023	10.196968	15.982899
H	36.698082	9.818361	15.452474
H	36.368343	10.126730	17.164880
C	35.090269	5.401767	16.291747
H	36.031899	5.229616	15.749735
H	34.620026	4.420647	16.435887
C	34.189685	6.302679	15.450160
H	33.999118	5.837133	14.474874
H	33.215847	6.414824	15.939683
C	34.826787	7.681842	15.252163
H	35.484462	7.672455	14.369172
H	34.052329	8.426921	15.021972
C	36.788825	7.982186	18.588443
H	36.412810	7.758537	19.586774
C	37.932240	8.717786	18.483634
H	38.358702	8.859991	17.495011
C	38.584457	9.380996	19.592480
C	37.897225	9.397753	20.923649
H	38.046354	8.441013	21.437937
H	36.821248	9.552481	20.828618
H	38.298615	10.184422	21.559558
C	39.791786	10.039915	19.514401
H	40.072293	10.644949	20.372931
C	40.747995	9.979014	18.472614
H	40.570029	9.280459	17.663007
C	41.900856	10.727356	18.482159
H	42.038405	11.448384	19.284972
C	42.933826	10.653732	17.507804
C	42.905127	9.560745	16.460708
H	42.521459	9.927850	15.500991
H	42.291130	8.716201	16.773293
H	43.904831	9.166742	16.278291
C	43.937183	11.623379	17.527941
H	43.934964	12.398601	18.291600
C	44.949602	11.633477	16.565746
H	45.003680	10.811227	15.857496

Model 8: Monkey PSB13

N	45.743683	12.223677	16.613009
H	46.234174	12.757494	17.354768
H	46.242656	12.176818	15.717281
C	35.227965	7.891380	17.053247
C	34.915268	6.428292	17.450478
C	34.091991	6.439466	18.757158
H	33.767676	5.420596	19.000486
H	33.203918	7.071115	18.660942
H	34.672256	6.809669	19.604665
C	36.209107	5.613701	17.675632
H	36.787677	5.517709	16.750355
H	35.962094	4.604814	18.026489
H	36.856036	6.070767	18.431508
C	34.756261	8.462406	15.912099
C	34.772826	9.943465	15.628660
H	35.483060	10.196169	14.828240
H	35.004278	10.539362	16.512991
H	33.783436	10.257690	15.273873
C	34.068866	5.740080	16.363479
H	33.034128	6.064401	16.490804
H	34.088923	4.654637	16.510147
C	34.482644	6.147762	14.956749
H	35.557760	5.987838	14.809123
H	33.959041	5.553342	14.199370
C	34.154639	7.629060	14.807907
H	34.516318	8.026022	13.850721
H	33.058715	7.754435	14.802531
C	36.095899	8.587604	17.988121
H	36.085691	8.228066	19.012401
C	37.060339	9.483262	17.636408
H	37.130111	9.802271	16.600965
C	38.183491	9.822689	18.457948
C	38.263638	9.290428	19.868019
H	38.553149	8.232402	19.863545
H	37.289744	9.354455	20.359464
H	38.970229	9.841996	20.486140
C	39.235028	10.468326	17.828507
H	39.047313	10.890013	16.849156
C	40.548961	10.408661	18.319873
H	40.630578	9.991657	19.312914
C	41.736387	10.752674	17.700434
H	41.728627	11.250144	16.733450
C	42.952414	10.576522	18.409610
C	42.892627	9.726692	19.646471
H	42.233013	8.876473	19.500204
H	42.528648	10.326785	20.485116
H	43.871466	9.328452	19.894127
C	44.188928	11.172436	18.116037
H	44.878446	11.331083	18.946698
C	44.639174	11.529232	16.846722
H	44.121050	11.136571	15.971498

Model 9: Squid PSB11

51 Atoms

N	9.796233	38.054782	57.858373
H	8.874230	38.327781	58.190451
H	9.949860	37.043264	57.784239
C	17.131212	44.828289	61.316098
C	18.532048	44.846576	60.654834
C	18.870817	46.259227	60.126053
H	19.906116	46.277020	59.772084
H	18.779472	47.006821	60.922821
H	18.237644	46.559165	59.284186
C	18.548568	43.860266	59.463264
H	18.399492	42.824057	59.788053

H	19.506550	43.917572	58.932764
H	17.755349	44.100632	58.751135
C	16.912775	44.359680	62.574668
C	15.608993	44.463847	63.332561
H	15.119096	43.483846	63.410627
H	14.902069	45.168229	62.891403
H	15.819203	44.788952	64.362000
C	19.631556	44.455889	61.667449
H	19.860961	45.321078	62.302797
H	20.550740	44.232709	61.115124
C	19.220124	43.289667	62.561279
H	18.961602	42.416279	61.948123
H	20.049083	42.987873	63.210366
C	18.004888	43.701138	63.388020
H	17.572340	42.835050	63.909033
H	18.305715	44.399838	64.183154
C	16.029066	45.291883	60.462118
H	16.203974	46.156939	59.824983
C	14.869973	44.599724	60.325323
H	14.771476	43.680386	60.893245
C	13.772753	44.876468	59.427957
C	13.645232	46.232245	58.791031
H	14.483039	46.425287	58.111967
H	13.676323	47.020597	59.551211
H	12.721317	46.331297	58.215712
C	12.925458	43.821423	59.175028
H	13.167594	42.897372	59.686577
C	11.761487	43.797790	58.360372
H	11.313150	44.752256	58.089777
C	11.061109	42.678445	57.961636
H	10.061518	42.853916	57.567039
C	11.469136	41.306496	57.959251
C	12.906167	40.878555	58.117623
H	13.087954	40.474542	59.121559
H	13.595416	41.701705	57.942621
H	13.152791	40.094901	57.395900
C	10.472504	40.349016	57.793664
H	9.437313	40.675394	57.796475
C	10.729282	38.979201	57.692339
H	11.721453	38.619755	57.440379

Model 10: Squid PSB7

51 Atoms

N	10.218705	37.736803	58.236299
H	9.336885	37.967997	58.686761
H	10.436916	36.734440	58.188354
C	17.077790	45.805691	61.088780
C	18.542639	45.801461	60.572966
C	19.003711	47.245689	60.276124
H	20.081059	47.248075	60.087677
H	18.803547	47.906515	61.126262
H	18.524467	47.653210	59.380497
C	18.670479	44.995114	59.258450
H	18.547541	43.917602	59.418410
H	19.664126	45.151007	58.825743
H	17.931084	45.319843	58.520122
C	16.711991	45.275801	62.284011
C	15.342046	45.412273	62.907099
H	14.820596	44.445021	62.930403
H	14.698981	46.133474	62.402649
H	15.451300	45.729104	63.954201
C	19.506350	45.212286	61.628135
H	19.755013	45.987394	62.359377
H	20.449342	44.949675	61.134031
C	18.920609	44.019543	62.377597
H	18.657104	43.218029	61.674029
H	19.661441	43.602867	63.069356
C	17.668731	44.464046	63.133024
H	17.124700	43.592856	63.525928
H	17.945947	45.054196	64.021193
C	16.097694	46.496130	60.222618
H	16.342752	47.521999	59.969678
C	14.938331	46.042487	59.671907
H	14.322878	46.776959	59.154433
C	14.478997	44.673323	59.585263
C	15.460119	43.578807	59.927198
H	15.316114	43.230031	60.952929
H	16.480261	43.926652	59.837239
H	15.355214	42.723517	59.263715
C	13.213906	44.370774	59.109831
H	12.518907	45.172875	58.870128
C	12.878935	43.015315	58.863131
H	13.689541	42.354388	59.108269
C	11.793803	42.330247	58.374274
H	10.826629	42.798064	58.199143
C	11.949846	40.926632	58.121342
C	13.334755	40.335909	57.969581
H	13.589283	39.670983	58.801373
H	14.109270	41.090276	57.878806
H	13.384199	39.762586	57.041472
C	10.858436	40.066047	58.065390
H	9.859580	40.440506	58.259842
C	11.077802	38.691642	57.920271
H	12.027209	38.346034	57.524220

Model 11: Squid PSB9

N	9.641240	37.839875	58.242409
H	8.755961	38.154885	58.630621
H	9.758010	36.822561	58.196789
C	16.701321	44.908891	61.160378
C	18.126597	44.775513	60.570010
C	18.862597	46.136369	60.625767
H	18.935428	46.532940	61.642884
H	18.340672	46.880571	60.015614
H	19.876704	46.041507	60.219301
C	18.078741	44.326397	59.097451
H	17.607375	45.076333	58.456838
H	17.527875	43.385301	58.985571
H	19.097418	44.167531	58.723718
C	16.417634	44.586627	62.450524
C	15.074071	44.775608	63.114428
H	15.222563	45.190906	64.120030
H	14.566789	43.810092	63.238949
H	14.403419	45.441538	62.571497
C	18.906501	43.699551	61.352786
H	18.478797	42.714399	61.118312
H	19.943136	43.690647	60.994830
C	18.878107	43.932433	62.856863
H	19.447064	43.153480	63.377164
H	19.388603	44.875715	63.065701
C	17.444271	43.990212	63.391697
H	17.092261	42.981657	63.653935
H	17.417289	44.548369	64.339685
C	15.674652	45.437066	60.249493
H	15.952294	46.301812	59.645326
C	14.457387	44.868125	60.050992
H	14.239283	43.953777	60.593795
C	13.395834	45.384816	59.208196
C	13.431788	46.827410	58.800292
H	14.254442	46.985746	58.095153

H	13.599210	47.493632	59.651584
H	12.507963	47.119985	58.292965
C	12.351474	44.596304	58.778240
H	11.491301	45.068951	58.307278
C	12.392679	43.180206	58.803712
H	13.334424	42.743085	59.113154
C	11.396463	42.323839	58.410314
H	10.408150	42.722051	58.183060
C	11.588904	40.920142	58.269313
C	12.973317	40.328545	58.250166
H	13.139336	39.642134	59.086485
H	13.750716	41.087798	58.265271
H	13.104852	39.777728	57.314509
C	10.477953	40.090904	58.161724
H	9.485975	40.517982	58.263833
C	10.615713	38.709613	58.026389
H	11.565447	38.291043	57.709535
H	8.460786	42.325420	58.045126
C	9.864307	40.114841	57.545806
H	8.831627	40.077783	57.235433
C	10.462950	38.879993	57.738860
H	11.528177	38.757859	57.910560

Model 12: Squid PSB13

51 Atoms

N	9.726281	37.772140	57.708844
H	8.723798	37.822911	57.558779
H	10.078025	36.813916	57.746168
C	17.286597	44.602085	61.386465
C	18.726479	44.586777	60.823912
C	19.123658	45.993129	60.320693
H	20.175804	45.991301	60.019689
H	19.004435	46.741482	61.113102
H	18.538375	46.304403	59.448561
C	18.801753	43.599081	59.634933
H	18.599277	42.568937	59.950354
H	19.798878	43.627733	59.181349
H	18.073933	43.856242	58.860088
C	16.964207	44.176139	62.636945
C	15.604126	44.314442	63.284577
H	15.106740	43.338704	63.371505
H	14.934252	44.994544	62.756412
H	15.732623	44.690384	64.310299
C	19.741839	44.168209	61.910212
H	19.971382	45.035753	62.539658
H	20.683050	43.890857	61.423923
C	19.223850	43.042836	62.802449
H	18.956860	42.168549	62.193976
H	19.999817	42.717484	63.502424
C	17.981755	43.526590	63.546693
H	17.490906	42.696468	64.074842
H	18.258062	44.249317	64.328991
C	16.238392	45.016912	60.441158
H	16.381553	45.913301	59.839384
C	15.171272	44.209335	60.223770
H	15.163416	43.276260	60.778397
C	14.058997	44.371766	59.322196
C	13.798505	45.695446	58.659428
H	14.625800	45.957763	57.989592
H	13.751353	46.498747	59.402446
H	12.873193	45.693494	58.076996
C	13.314334	43.229197	59.125453
H	13.690943	42.341201	59.619817
C	12.118631	43.013188	58.409476
H	11.592402	43.861806	57.981925
C	11.604373	41.737365	58.280661
H	12.221333	40.920835	58.650432
C	10.349520	41.408919	57.725876
C	9.337132	42.472759	57.405993
H	8.971604	42.362571	56.384847
H	9.705028	43.483125	57.558545