

Supporting Information for
“Spectral Tuning of Deep Red Cone Pigments”

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This section provides the literature sources for the absorption maxima of the A1 and A2 vertebrate M/LWS pigments as well as additional details regarding the theoretical methods. Our principal conclusion is that the deep red pigments achieve an enhanced bathochromic shift by selecting a *6-s-trans* conformation of the bound chromophore. Those pigments which are predicted to adopt a *6-s-trans* A2 chromophore are indicated in solid rectangles. We consider these assignments compelling. Those pigments which are predicted to adopt a *6-s-trans* A1 chromophore are indicated in dashed rectangles. We consider these assignments tentative. All the other pigments shown have *6-s-cis* A1 or A2 chromophores.

Over 200 absorption maxima of vertebrate M/LWS pigments from various literature sources are collected in Tables S1 (A1 chromophores) and S2 (A2 chromophores). These data were used to generate the histograms shown in Figure 3.

The isolated chromophore models that we used to examine the effect of *6-s-cis* versus *6-s-trans* conformation on the electronic properties of the isolated chromophores are shown in Tables S3 and S4. The ground state geometries of the models were minimized by DFT methods in Gaussian-03 (29). The B3LYP/6-31G(d) Hamiltonian was selected. The excited state properties were calculated by using MNDO-PSDCI theory (30-33). The molecular diagram that is shown to the left of the data shows the geometry of the chromophore with the lowest energy conformation. In general, protonated Schiff bases without counterions select the *6-s-trans*. Most others select *6-s-cis*.

Table S1: The absorption maxima of various A1-containing vertebrates collected from literature data. These data were used to generate the histograms in Figure 3.

λ_{\max}	Origin of A1 Pigment	Reference
440	European ground squirrel (<i>Citellus citellus</i>)	(34)
502	Frog (<i>Xenopus laevis</i>)	(35)
503	Blue tit (<i>Parus caeruleus</i>)	(36)
505	Rudd (summer) (<i>Scardinius erythrophthalmus</i>)	(37)
508	Mouse	(38)
510	Mouse	(39)
511.6	<i>Batrachocottus nicolski</i> (300-1000 m)	(40)
512	Wolf-eel (<i>Anarrhichthys ocellatus</i>)	(41)
512.3	<i>Limnocottus eurystomus</i> (100-500 m)	(40)
512.6	<i>Asprocottus intermedius</i> (100-500 m)	(40)
513	Dwarf wrymouth (<i>Lyconectes aleutensis</i>)	(41)
513	English sole (<i>Parophrys vetula</i>)	(41)
513	Great sculpin (<i>Myoxocephalus polyacanthocephalus</i>)	(41)
513	Grunt sculpin (<i>Rhamphocottus richardsoni</i>)	(41)
513	Lingcod (<i>Ophiodon elongatus</i>)	(41)
513	Rock prickpleback (<i>Xiphister mucosus</i>)	(41)
514	Pacific sandfish (<i>Trichodon trichodon</i>)	(41)
516	Coral fish (<i>Dascyllus trimaculatus</i>)	(42)
516	Guinea pig (<i>Cavia porcellus</i>)	(43)
516	Kelp greenling (<i>Hexagrammos decagrammus</i>)	(41)
516	Pudget sound sculpin (<i>Artidius meanyi</i>)	(41)
517	Guillfish (<i>Ptilichthys goodei</i>)	(41)
517.3	<i>Batrachocottus multiradiatus</i> (100-500 m)	(40)
519	Great sculpin (<i>Myoxocephalus polyacanthocephalus</i>)	(41)
519	Pudget sound sculpin (<i>Artidius meanyi</i>)	(41)
519	White-spotted greenling (<i>Hexagrammos stelleri</i>)	(41)
519	Young larval flounder	(44)
520	Brown rockfish (<i>Sebastes auricaulatus</i>)	(41)
520	Walleye pollock (<i>Theragra chalcogramma</i>)	(41)
520	White-spotted greenling (<i>Hexagrammos stelleri</i>)	(41)
520.6	<i>Cottocomephorus inermis</i> (50-450 m)	(40)
521	Brown rockfish (<i>Sebastes auricaulatus</i>)	(41)
521	<i>Batrachocottus baicalensis</i> (1-120 m)	(40)
521	House gecko (<i>Hemidactylus garnotii</i>)	(45)
521	Pacific herring (<i>Clupea pallasii</i>)	(41)
521	Tokay Gecko (<i>Gecko gecko</i>)	(46)
521.2	<i>Paracottus kneri</i> (2-5 m)	(40)

Table S1 continued

522	Pacific herring (<i>Clupea pallasii</i>)	(41)
522	West Australian dhufish (<i>Glaucosoma hebraicum</i>)	(47)
522	White-spotted greenling (<i>Hexagrammos stelleri</i>)	(41)
522.6	<i>Paracottus kneri</i> (2-5 m)	(40)
523.3	<i>Cottocomephorus grewingki</i> (1-300 m)	(40)
524	Dolphin (bottlenose) (<i>Tursiops truncatus</i>)	(48)
524	Kelp greenling (<i>Hexagrammos decagrammus</i>)	(41)
525	Baikal Cottoids-shallow water	(40)
525	<i>Cottus kessleri</i> (2-5 m)	(40)
525	Hawaiian saddle wrasse (<i>Thalassoma duperrey</i>)	(49)
526	Mediterranean gecko (<i>Hemidactylus turcicus</i>)	(45)
526	Pink surfperch (<i>Zalembeus rosaceus</i>)	(50)
527	Pacific sand lance (<i>Ammodytes hexapterus</i>)	(41)
528	Weever fish (<i>Trachinus vipera</i>)	(51)
529	Northern anchovy (<i>Engraulis mordax</i>)	(41)
529	Shiner surfperch (<i>Cymatogaster aggregata</i>)	(50)
530	Cave fish (<i>Astyanax fasciatus</i>)	(52)
530	Chimpanzee (<i>Pan troglodytes</i>)	(53)
530	Guinea pig (<i>Cavia porcellus</i>)	(54)
530	Human (<i>Homo sapiens</i>)	(55)
530	Northern anchovy (<i>Engraulis mordax</i>)	(41)
530	Tammar wallaby (<i>Macropus eugenii</i>)	(56)
530.7	Diana monkey (<i>Cercopithecus diana</i>)	(57)
531	Deer (<i>Odocoileus virginianus</i>)	(43)
531	Rainbow trout (<i>Oncorhynchus mykiss</i>)	(58)
531	Winter adult flounder (<i>Pseudopleuronectes americanus</i>)	(44)
532	American/squirrel monkey (<i>Saimuri sciureus</i>)	(59)
532	Coral fish (<i>Pomacentrus coelestis</i>)	(60)
532	Squirrel (<i>Sciurus carolinensis</i>)	(43)
533	Guppy (<i>Poecilia reticulata</i>)	(61)
533	Malawi cichlid fish (<i>Metriacroma zebra</i>)	(62)
533	Moustached guenon (<i>Cercopithecus cephus</i>)	(57)
533	Patas monkey (<i>Erythrocebus patas</i>)	(57)
533	Scinc gecko (<i>Teratoscincus scincus</i>)	(45)
533.3	<i>Cercopithecus talapoin</i>	(57)
533.9	Spot-nosed monkey (<i>Cercopithecus petaurista</i>)	(57)
534	Blind mole rat (<i>Spalax ehrenbergi</i>)	(63)
535	Black bream (<i>Acanthopagrus butcheri</i>)-young	(64)
535	Fat-tailed dunnart (<i>Sminthopsis crassicaudata</i>)	(65)
535	Grivet (<i>Cercopithecus aethiops</i>)	(57)
535.2	<i>Papio papio</i> (ii)	(57)

Table S1 continued

535.6	<i>Papio papio</i> (iv)	(57)
536	American/squirrel monkey (<i>Saimuri sciureus</i>)	(66)
536	<i>Dimidiochromis compressiceps</i>	(62)
536	Epigeal fish (<i>Astyanax fasciatus</i>)	(67)
536	Rhesus macaque (<i>Macaca mulatta</i>)	(57)
536.4	<i>Papio papio</i> (i)	(57)
537	White-tailed deer (<i>Odocoileus virginiana</i>)	(68)
538.8	<i>Papio papio</i> (iii)	(57)
539	Horse (<i>Equus caballus</i>)	(69)
539	Marmoset (New world monkey) (<i>Callithrix jacchus</i>)	(43)
540	Ring-tailed lemur (<i>Lemur catta</i>)	(70)
541	Kelp greenling (<i>Hexagrammos decagrammus</i>)	(41)
541	Saddle-backed tamarin (<i>Saguinus fuscicollis</i>)	(59)
42	Fallow deer (<i>Dama dama</i>)	(68)
543	Owl monkey (<i>Aotus trivirgatus</i>)	(71)
543	Penguin (<i>Spheniscus humboldti</i>)	(36)
544	Golden lion tamarin (<i>Leontopithecus rosalia rosalia</i>)	(72)
545	Black bream (<i>Acanthopagrus butcheri</i>)-adult	(64)
545	Golden-handed tamarin (<i>Saguinus midis</i>)	(72)
545	Horse (<i>Equus caballus</i>)	(43)
545	Saddle-backed tamarin (<i>Saguinus fuscicollis</i>)	(73)
546	Cotton top tamarin (<i>Saguinus oedipus</i>)	(72)
546	<i>Cottus kessleri</i> (2-5 m)	(40)
547	American/squirrel monkey (<i>Saimuri Sciureus</i>)	(59)
547	Ring-tailed lemur (<i>Lemur catta</i>)	(72)
547	Winter adult flounder (<i>Pseudopleuronectes americanus</i>)	(44)
548.3	Zebrafish (<i>Danio rerio</i>)	(74)
549	American/squirrel monkey (<i>Saimuri sciureus</i>)	(66)
549	Boa constrictor imperator	(75)
549	Dusky titi (<i>Callicebus moloch</i>)	(73)
551	Ball python (<i>Python regius</i>)	(76)
552	Sheep (<i>Ovis aries</i>)	(68)
553	Cat (<i>Felis catus</i>)	(43)
553	Goat (<i>Capra hircus</i>)	(68)
553	Marmoset (New world monkey) (<i>Callithrix jacchus</i>)	(43)
554	Garter Snake (<i>Thamnophis sirtalis</i>)	(76)
554	Golden lion tamarin (<i>Leontopithecus rosalia rosalia</i>)	(72)
554	White-spotted greenling (<i>Hexagrammos stelleri</i>)	(41)
555	Arctic fox (<i>Alopex lagopus</i>)	(71)

Table S1 continued

555	Cow/Bovine (<i>Bos taurus</i>)	(68)
555	Domestic dog (<i>Canis familiaris</i>)	(71)
555	Island gray foxes (<i>Urocyon littoralis</i>)	(71)
555	Lamprey	(35)
555	Red foxes (<i>Vulpes vulpes</i>)	(71)
555	Tawny Owl (<i>Strix aluco</i>)	(36)
555	Tree Shew (<i>Tupaia belangeri</i>)	(77)
556	Blackbird (<i>Turdus merula</i>)	(78)
556	Saddle-backed tamarin (<i>Saguinus fuscicollis</i>)	(59)
557	Blackbird (<i>Turdus merula</i>)	(36)
557	Cotton top tamarin (<i>Saguinus oedipus</i>)	(72)
557	Frog (<i>Xenopus laevis</i>)	(52)
557	Golden-handed tamarin (<i>Saguinus midis</i>)	(72)
557	Honey possum (<i>Tarsipes rostratus</i>)	(65)
557	Pig (<i>Sus scrofa</i>)	(68)
557	Saddle-backed tamarin (<i>Saguinus fuscicollis</i>)	(73)
557.7	Zebrafish (<i>Danio rerio</i>)	(74)
558	Cave fish (<i>Astyanax fasciatus</i>)	(52)
558	White-spotted greenling (<i>Hexagrammos stelleri</i>)	(41)
560	American chameleon (regenerated)	(79)
560	Chameleon (<i>Anolis</i>)	(79)
560	Chimpanzee (<i>Pan troglodytes</i>)	(53)
560	Cyprinid fish (<i>Danio aequipinnatus</i>)	(80)
560	Human (<i>Homo sapiens</i>)	(81)
560	Laughing gull (<i>Larus atricilla</i>)	(36)
560	Zebrafinch (<i>Taeniopygia guttata</i>)	(81)
561	American/squirrel monkey (<i>Saimuri sciureus</i>)	(59)
561	Chameleon (<i>Anolis</i>)	(52)
561	Dusky titi (<i>Callicebus moloch</i>)	(73)
561	Marmoset (New world monkey) (<i>Callithrix jacchus</i>)	(43)
561.5	Rhesus macaque (<i>Macaca mulatta</i>)	(57)
562	Lingcod (<i>Ophiodon elongatus</i>)	(41)
562	Saddle-backed tamarin (<i>Saguinus fuscicollis</i>)	(73)
562	White-headed munia (<i>Louchura maja</i>)	(36)
562.7	Spot-nosed monkey (<i>Cercopithecus petaurista</i>)	(57)
563	Blue tit (<i>Parus caeruleus</i>)	(36)
563	Cotton top tamarin (<i>Saguinus oedipus</i>)	(72)
563	Cut-throat finches (<i>Amadina fasciata</i>)	(36)
563	European Starling (<i>Sturnus vulgaris</i>)	(36)
563	Gouldian finch (<i>Erythrura gouldiae</i>)	(36)
563	House sparrow (<i>Passer domesticus</i>)	(36)
563	Mummichog killifish (<i>Fundulus heteroclitus</i>)	(82)

Table S1 continued

563	Plum-headed finch (<i>Neochmia modesta</i>)	(83)
563	Saddle-backed tamarin (<i>Saguinus fuscicollis</i>)	(72)
563	Turkey (<i>Meleagris galoparco</i>)	(36)
563	White-headed munia (<i>Louchura maja</i>)	(83)
564	American/squirrel monkey (<i>Saimuri sciureus</i>)	(66)
564	Brushland tinamou (<i>Nothoprocta cinerascens cinerascens</i>)	(36)
564	Budgerigar (parakeet) (<i>Melospiza undulatus</i>)	(36)
564	<i>Cercopithecus talapoin</i>	(57)
564	Cut-throat finches (<i>Amadina fasciata</i>)	(83)
564	Gouldian finch (<i>Erythrura gouldiae</i>)	(83)
564	Plum-headed finch (<i>Neochmia modesta</i>)	(83)
564	White-headed munia (<i>Louchura maja</i>)	(83)
564	Zebrafish (<i>Danio rerio</i>)	(84)
564.3	<i>Papio papio</i> (i)	(57)
564.4	<i>Papio papio</i> (iii)	(57)
565	Blue tit (<i>Parus caeruleus</i>)	(78)
565	Gouldian finch (<i>Erythrura gouldiae</i>)	(83)
565	Plum-headed finch (<i>Neochmia modesta</i>)	(36)
565	Rook (<i>Corvus frugilegus</i>)	(36)
565	Rudd (summer) (<i>Scardinius erythrophthalmus</i>)	(37)
565.3	Moustached guenon (<i>Cercopithecus cephus</i>)	(57)
565.7	<i>Papio papio</i> (ii)	(57)
565.9	Diana monkey (<i>Cercopithecus diana</i>)	(57)
566	Chilean tinamou (<i>Nothoprocta perdicaria sanborni</i>)	(36)
566	Epigeal fish (<i>Astyanax fasciatus</i>)	(67)
566	Peacock /Peafowl (<i>Pavo cristatus</i>)	(36)
566.3	Grivet (<i>Cercopithecus aethiops</i>)	(57)
566.3	Patas monkey (<i>Erythrocebus patas</i>)	(57)
567	Emu (<i>Dromiceius novae-hollandiae</i>)	(36)
567	Japanese quail (<i>Coturnix japonica</i>)	(36)
567	Mallard duck (<i>Anas platyrhynchos</i>)	(36)
567	Pacific sandfish (<i>Trichodon trichodon</i>)	(41)
567	Pekin robin (<i>Lotothrix lutea</i>)	(36)
567	Rock dove (Feral pigeon) (<i>Columba livia</i>)	(36)
567	Zebrafinch (<i>Taeniopygia guttata</i>)	(36)
567.8	<i>Papio papio</i> (iv)	(57)
568	Red Irish lord (<i>Hemilepidotus hemilepidotus</i>)	(41)
569	Cabezon (<i>Scorpaenichthys marmoratus</i>)	(41)
569	<i>Dimidiochromis compressiceps</i>	(62)
570	Aylesbury duck (<i>Anas platyrhynchos domesticus</i>)	(36)
570	Chicken (<i>Gallus gallus</i>)	(36)

Table S1 continued

570	Hawaiian saddle wrasse (<i>Thalassoma duperrey</i>)	(49)
570	Khaki Campbell duck (<i>Anas platyrhynchos domesticus</i>)	(36)
570	Ostrich (<i>Strutio camelus</i>)	(36)
570	Rhea (<i>Rhea americana</i>)	(36)
571	Canary (<i>Serinus canaria</i>)	(36)
571	Ornate dragon lizards (<i>Ctenophorus ornatus</i>)	(85)
572	Giant danio (<i>Danio malabaricus</i>)	(42)
572	Guppy (<i>Poecilia reticulata</i>)	(61)
574	Dwarf wrymouth (<i>Lyconectes aleutensis</i>)	(41)
574	Rainbow trout (<i>Oncorhynchus mykiss</i>)	(58)
575	Black bream (<i>Acanthopagrus butcheri</i>)-adult	(64)
575	Frog (<i>Xenopus laevis</i>)	(35)
575	Laughing gull (<i>Larus atricilla</i>)	(36)
575	Salamander	(86)
582	Saddle-backed tamarin (<i>Saguinus fuscicollis</i>)	(59)
584	Pacific herring (<i>Clupea pallasii</i>)	(41)

Table S2: The absorption maxima of various A2-containing vertebrate visual pigments. These data were used to generate Figure 3.

λ_{\max}	Origin of A2 Pigment	Reference
515	Red-eared turtle (<i>Trachemys scripta</i>)	(87)
515	Rudd (winter) (<i>Scardinius erythrophthalmus</i>)	(37)
515	Southern hemisphere lamprey (<i>Geotria australis</i>)	(88)
521	Shovelnose sturgeon (<i>Scaphirhynchus platyrhynchus</i>)	(89)
525	Sea lamprey (upstream migrant) (<i>Petromyzon marinus</i>)	(90)
527	Frog (<i>Xenopus laevis</i>)	(35)
530	Freshwater turtle	(87)
531	Kelp surfperch (<i>Brachyistius frenatus</i>)	(50)
531	Kissing gourami (<i>Helostoma temminckii</i>)	(91)
531	Rainbow surfperch (<i>Hypsurus caryi</i>)	(50)
532	Adult green sunfish (native retina)	(92)
532	Goldfish (<i>Carassius auratus</i>)	(42)
534	Adult green sunfish (regenerated retina)	(92)
534	Black surfperch (<i>Embiotoca jacksoni</i>)	(50)
535	Adult european perch (<i>Perca fluviatilis</i>)	(93)
535	Brown trout (<i>Salmo trutta</i>)	(94)
535	Paddlefish (<i>Polyodon spathula</i>)	(89)
536	Striped surfperch (<i>E. lateralis</i>)	(50)
538	Carp (<i>Cyprinus carpio</i>)	(95)
538	Reef surfperch (<i>Micrometrus aurora</i>)	(50)
539	White sturgeon (<i>Acipenser transmontanus</i>)	(96)
542	Striped bass (<i>Morone saxatilis</i>)	(97)
542	Sturgeon (boneless fish w/jaws) (<i>Acipenser stellatus</i>)	(98)
544	Pile surfperch (<i>Damalichthys vacca</i>)	(50)
545	Dwarf surfperch (<i>M. minimus</i>)	(50)
545	Siberian sturgeon (<i>Acipenser baeri</i>)	(99)
559	Goldfish (<i>Carassius auratus</i>)	(81)
560	Adult yellow perch (<i>Perca flavescens</i>)	(100)
567	Epigean fish (<i>Astyanax fasciatus</i>)	(67)
600	Brown trout (<i>Salmo trutta</i>)	(94)
600	Sea lamprey (upstream migrant) (<i>Petromyzon marinus</i>)	(90)
602	Silver dollar (<i>Metynnis argenteus</i>)	(91)
605	Striped bass (<i>Morone saxatilis</i>)	(97)
605	White sturgeon (<i>Acipenser transmontanus</i>)	(96)
607	Paddlefish (<i>Polyodon spathula</i>)	(89)
610	Rudd (winter) (<i>Scardinius erythrophthalmus</i>)	(37)

Table S2 continued

610	Shovelnose sturgeon (<i>Scaphirhynchus platyrhynchus</i>)	(89)
610	Southern hemisphere lamprey (<i>Geotria australis</i>)	(88)
611	Epigean fish (<i>Astyanax fasciatus</i>)	(67)
611	Tiger salamander (<i>Ambystoma tigrinum</i>)	(91)
613	Siberian sturgeon (<i>Acipenser baeri</i>)	(99)
613	Sturgeon (boneless fish w/jaws) (<i>Acipenser stellatus</i>)	(98)
614	Goldfish (<i>Carassius auratus</i>)	(57)
616	Southern hemisphere lamprey (<i>Geotria australis</i>)	(88)
617	Red-eared turtle (<i>Trachemys scripta</i>)	(87)
618	Adult green sunfish (regenerated retina)	(92)
619	Carp (<i>Cyprinus carpio</i>)	(95)
620	Adult european perch (<i>Perca fluviatilis</i>)	(93)
620	Adult green sunfish (native retina)	(92)
620	Adult yellow perch (<i>Perca flavescens</i>)	(100)
620	Freshwater turtle	(87)
620	Frog (<i>Xenopus laevis</i>)	(35)
620	Goldfish (<i>Carassius auratus</i>)	(42)
620	Salamander	(86)
622	Adult green sunfish (regenerated retina)	(92)
623	Adult green sunfish (regenerated retina)	(92)
623	Rainbow trout (<i>Oncorhynchus mykiss</i>)	(58)
625	American chameleon (<i>Anolis carolinensis</i>)	(79)
628	Silver dollar (<i>Metynnis argenteus</i>)	(91)
630	Kissing gourami (<i>Helostoma temminckii</i>)	(91)

Table S3: A1 chromophore models and the calculated properties.

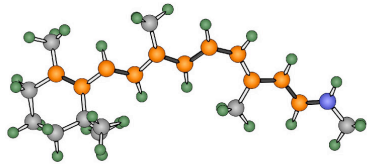
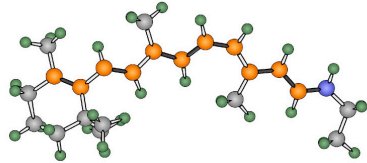
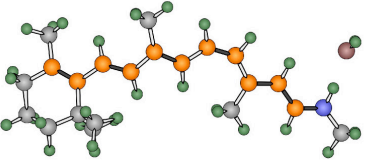
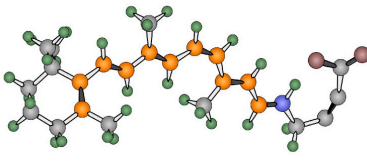
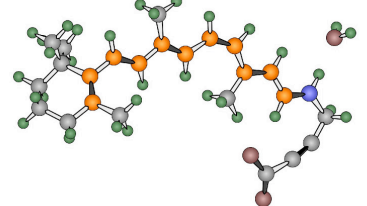
A1-methyl	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-874.0099487	-874.0106355
	ΔE_0 (kJ/mol)		-1.8033
	μ (Debye)	14.7942 D	12.2555 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	1.794	1.651
	$\Delta\Delta E_1(\text{cm}^{-1})$	1153.37	
A1-ethyl syn	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-913.3258308	-913.3263636
	ΔE_0 (kJ/mol)		-1.3987
	μ (Debye)	13.9217 D	11.444 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	1.859	1.702
	$\Delta\Delta E_1(\text{cm}^{-1})$	1266.29	
A1-methyl PSB with water	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-950.4403733	-950.4406926
	ΔE_0 (kJ/mol)		-0.8381
	μ (Debye)	17.1663 D	14.8810 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	1.944	1.778
	$\Delta\Delta E_1(\text{cm}^{-1})$	1338.88	
A1-asp up	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1138.2519527	-1138.2508251
	ΔE_0 (kJ/mol)		-2.9595
	μ (Debye)	19.3888 D	20.9135 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.916	2.686
	$\Delta\Delta E_1(\text{cm}^{-1})$	1855.07	
A1-asp down with water	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1214.6844769	-1214.6831974
	ΔE_0 (kJ/mol)		-3.3594
	μ (Debye)	17.7658 D	18.4510 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.803	2.652
	$\Delta\Delta E_1(\text{cm}^{-1})$	1217.90	

Table S3 continued

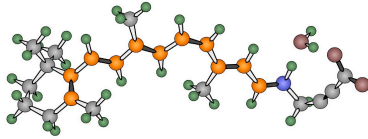
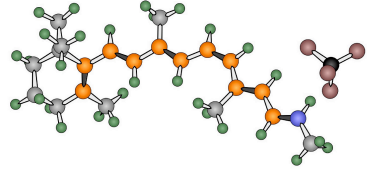
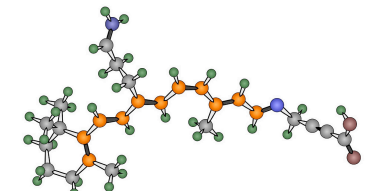
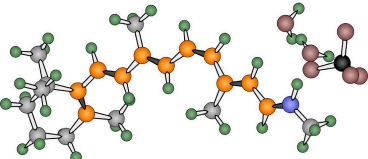
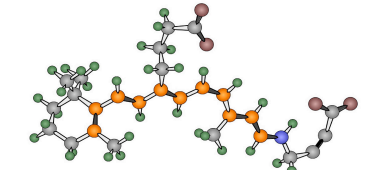
A1-asp up with water	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1214.7008698	-1214.6998068
	ΔE_0 (kJ/mol)	-2.7908	
	μ (Debye)	21.9301 D	23.4727 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.856	2.587
	$\Delta\Delta E_1(\text{cm}^{-1})$	2169.63	
A1-perchlorate	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1634.9331931	-1634.9316832
	ΔE_0 (kJ/mol)	-3.9642	
	μ (Debye)	16.3589 D	17.1504 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.808	2.547
	$\Delta\Delta E_1(\text{cm}^{-1})$	2105.11	
A1-9-NH ₂ asp up	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1271.4094225	-1271.4085495
	ΔE_0 (kJ/mol)	-2.2919	
	μ (Debye)	25.2682 D	26.8006 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	3.380	3.352
	$\Delta\Delta E_1(\text{cm}^{-1})$	225.84	
A1-perchlorate with 2 waters	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1787.8018522	-1787.8002316
	ΔE_0 (kJ/mol)	-4.2549	
	μ (Debye)	15.7714 D	16.8875 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.947	2.727
	$\Delta\Delta E_1(\text{cm}^{-1})$	1774.42	
A1-9-glu asp up	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1404.9008078	-1404.89898404
	ΔE_0 (kJ/mol)	-4.7882	
	μ (Debye)	31.3423 D	32.2276 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.613	2.450
	$\Delta\Delta E_1(\text{cm}^{-1})$	1314.68	

Table S4: A2 chromophore models and the calculated properties.

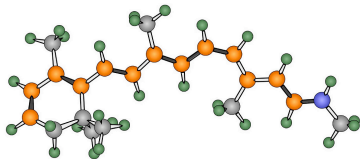
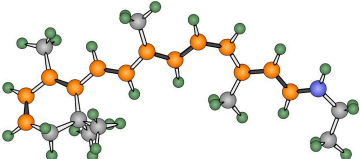
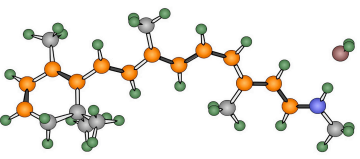
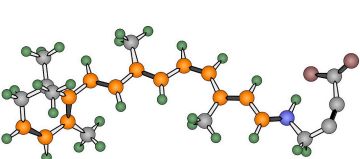
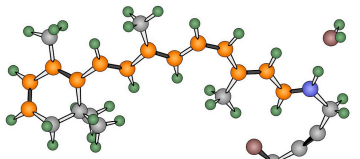
A2-methyl	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-872.7865914	-872.7877713
	ΔE_0 (kJ/mol)		-3.0978
	μ (Debye)	12.1218 D	10.4978 D
	$\Delta E_1[{}^1B_{0u}^+]$ (eV)	1.476	1.305
	$\Delta\Delta E_1(\text{cm}^{-1})$	1379.20	
A2-ethyl syn	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-912.1022548	-912.1033805
	ΔE_0 (kJ/mol)		-2.9553
	μ (Debye)	11.2412 D	9.7806 D
	$\Delta E_1[{}^1B_{0u}^+]$ (eV)	1.597	1.405
	$\Delta\Delta E_1(\text{cm}^{-1})$	1548.58	
A2-methyl PSB with water	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-949.2164011	-949.2173656
	ΔE_0 (kJ/mol)		-2.5322
	μ (Debye)	14.8141 D	13.2687 D
	$\Delta E_1[{}^1B_{0u}^+]$ (eV)	1.635	1.439
	$\Delta\Delta E_1(\text{cm}^{-1})$	1580.84	
A2-asp up	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1137.026897	-1137.0265942
	ΔE_0 (kJ/mol)		-0.7950
	μ (Debye)	19.8241 D	20.8899 D
	$\Delta E_1[{}^1B_{0u}^+]$ (eV)	2.784	2.530
	$\Delta\Delta E_1(\text{cm}^{-1})$	2048.64	
A2-asp down with water	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1213.4594536	-1216.4590649
	ΔE_0 (kJ/mol)		-7875.47
	μ (Debye)	17.9494 D	18.1190 D
	$\Delta E_1[{}^1B_{0u}^+]$ (eV)	2.554	2.320
	$\Delta\Delta E_1(\text{cm}^{-1})$	1887.33	

Table S4 continued

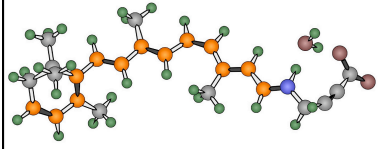
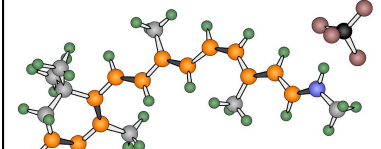
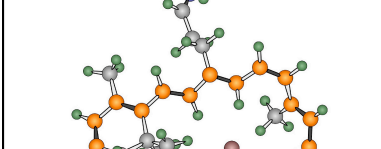
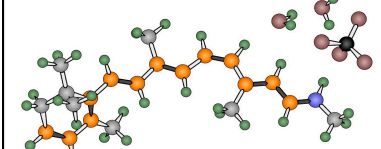
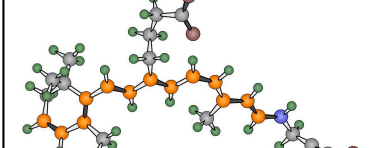
A2-asp up with water	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1213.4758777	-1213.4756560
	ΔE_0 (kJ/mol)	-0.5820	
	μ (Debye)	22.9928 D	23.0115 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.581	2.333
	$\Delta\Delta E_1(\text{cm}^{-1})$	2000.25	
A2-perchlorate	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1633.7088133	-1633.70740533
	ΔE_0 (kJ/mol)	-3.6966	
	μ (Debye)	17.3596 D	17.8056 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.525	2.357
	$\Delta\Delta E_1(\text{cm}^{-1})$	1355.01	
A2-9-NH ₂ asp up	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1270.1476897	-1270.1559854
	ΔE_0 (kJ/mol)		-21.7803
	μ (Debye)	28.0813 D	22.9090 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.543	2.207
	$\Delta\Delta E_1(\text{cm}^{-1})$	2710.02	
A2-perchlorate with 2 waters	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1786.5735044	-1786.5731929
	ΔE_0 (kJ/mol)	-0.8178	
	μ (Debye)	15.8846 D	16.7425 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.497	2.247
	$\Delta\Delta E_1(\text{cm}^{-1})$	2016.38	
A2-9-glu asp up	Property	6-s-cis	6-s-trans
	E_0 (Hartree)	-1403.6731944	-1403.6716429
	ΔE_0 (kJ/mol)	-4.0734	
	μ (Debye)	35.1945 D	35.7364 D
	$\Delta E_1[{}^1B_u^+]$ (eV)	2.255	2.229
	$\Delta\Delta E_1(\text{cm}^{-1})$	209.70	

Table S5: Comparison of residues at positions 164, 261, and 269 in selected red cone pigments found in regions 1 and 3 for the histogram of Figure 3.

A1 M/LWS	λ_{\max} (in nm)	Residue 164	Residue 261	Residue 269
<i>Region 1</i>				
Mouse	510	Ala	Tyr	Thr
Guinea Pig	516	Ser	Tyr	Ala
Rabbit	520	Ala	Tyr	Thr
Bottle-nosed Dolphin	524	Ala	Tyr	Thr
Human Green	531	Ala	Phe	Ala
<i>Region 3</i>				
Cavefish	558	Ser	Tyr	Thr
Human Red	560	Ser	Tyr	Thr
Zebrafinch	560	Ser	Tyr	Thr
Iodopsin	570	Ser	Tyr	Thr
Canary	571	Ser	Tyr	Thr

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