

## <sup>1</sup> Supplementary Materials



Figure 1: SIMMAP Tentilla presence/absence.

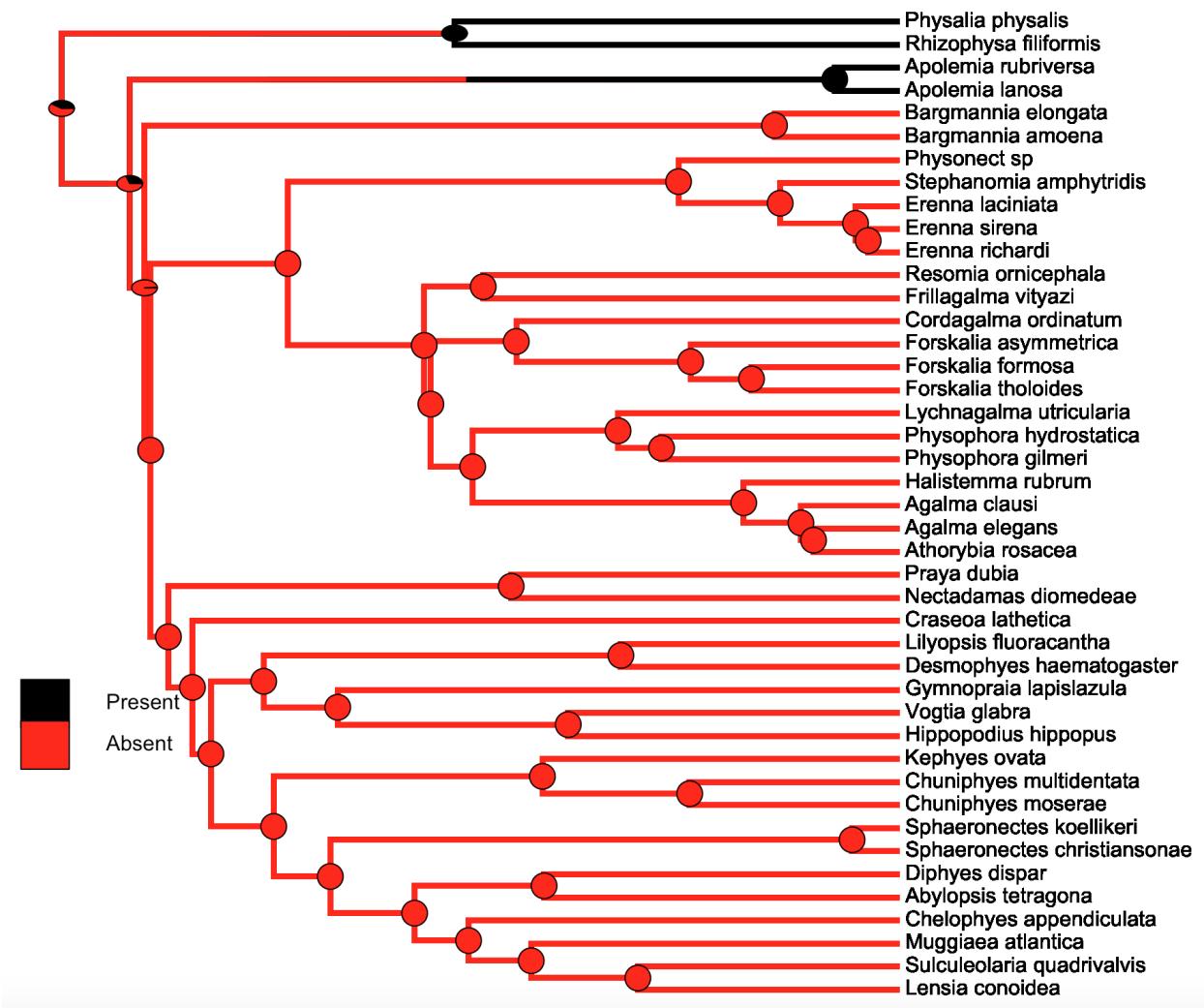


Figure 2: SIMMAP Cnidoband proximal heteroneme presence/absence.



Figure 3: SIMMAP Desmoneme+Rhopaloneme presence/absence.

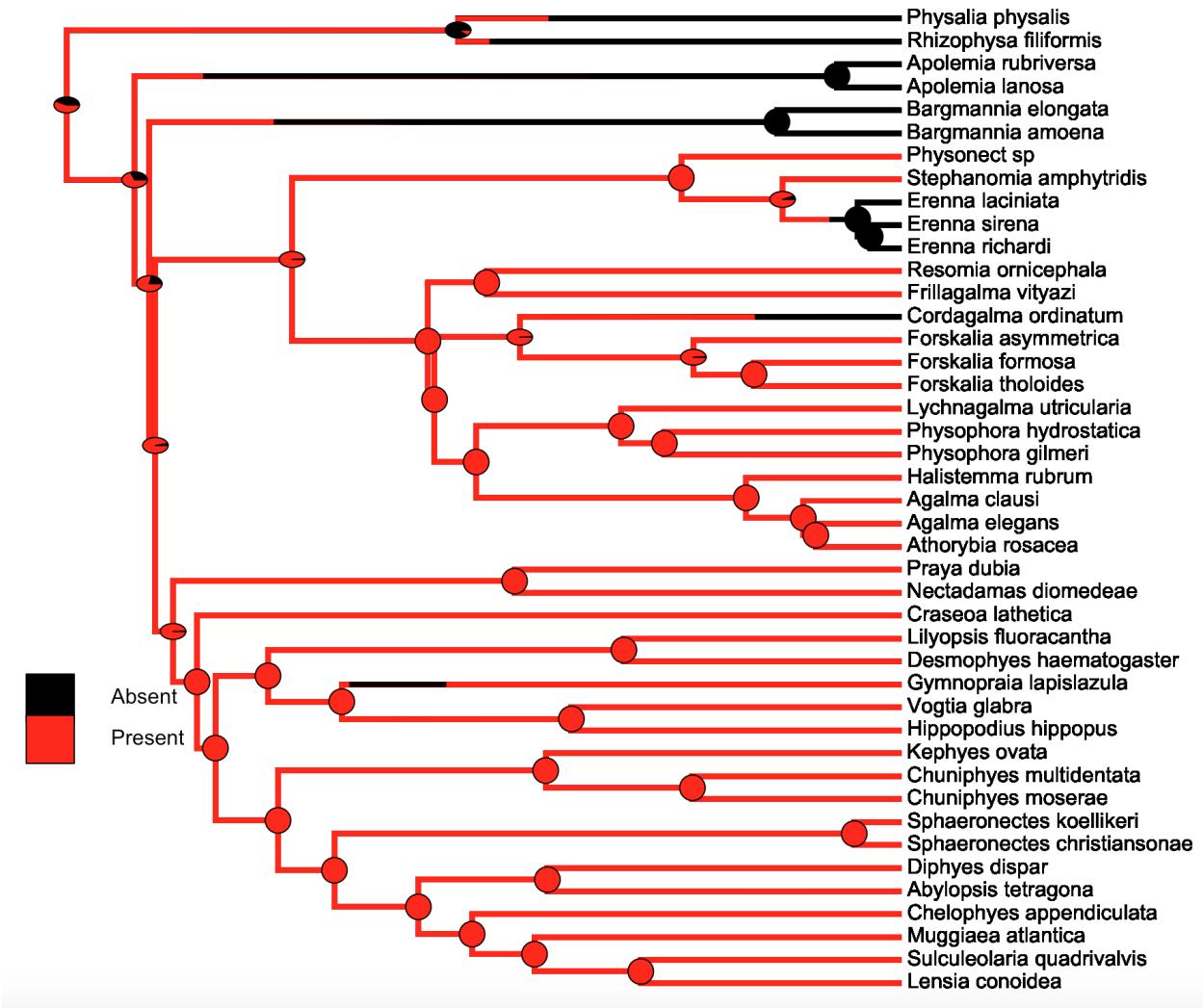


Figure 4: SIMMAP Actively discharging cnidobands presence/absence.

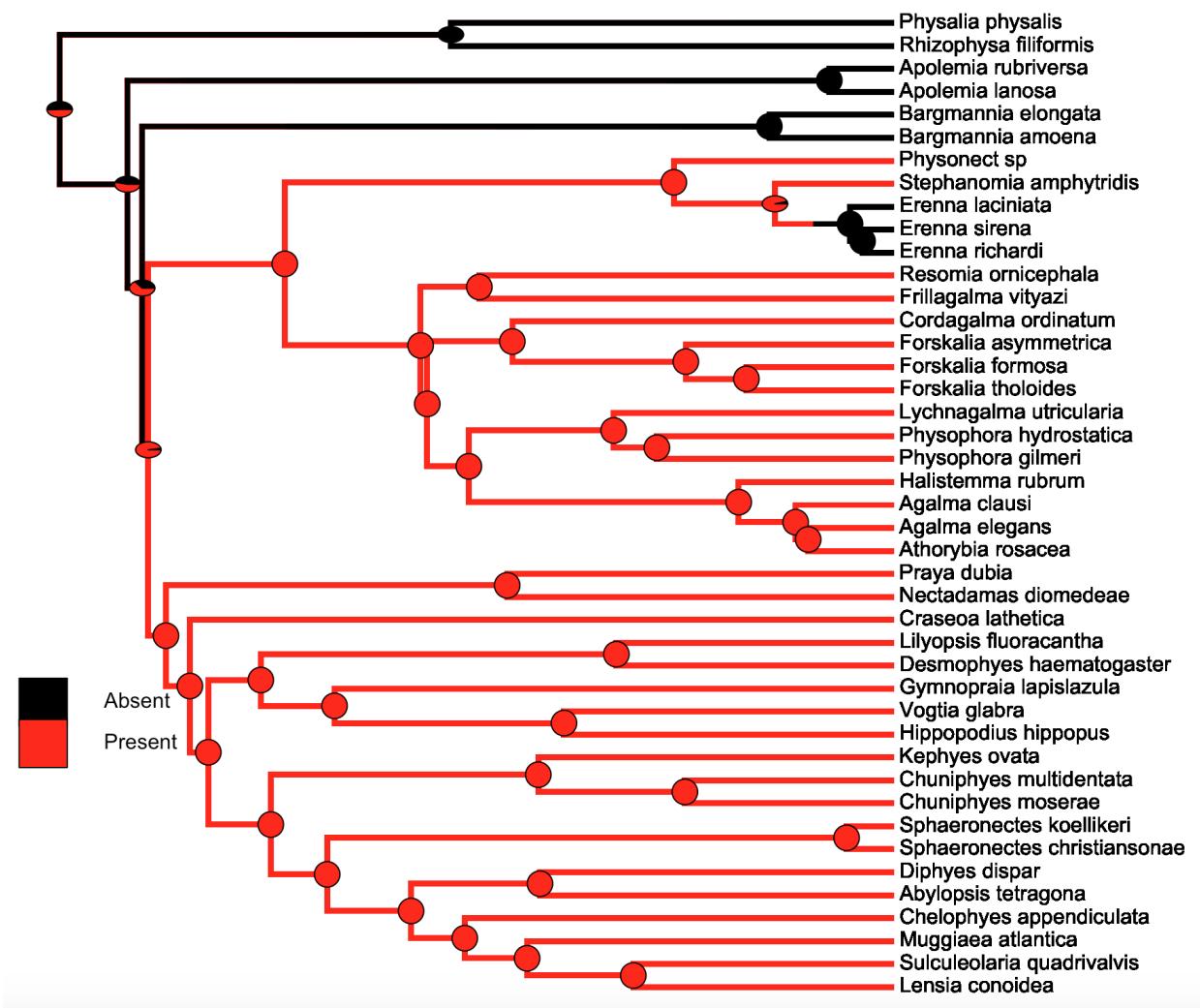


Figure 5: SIMMAP Elastic strands presence/absence.

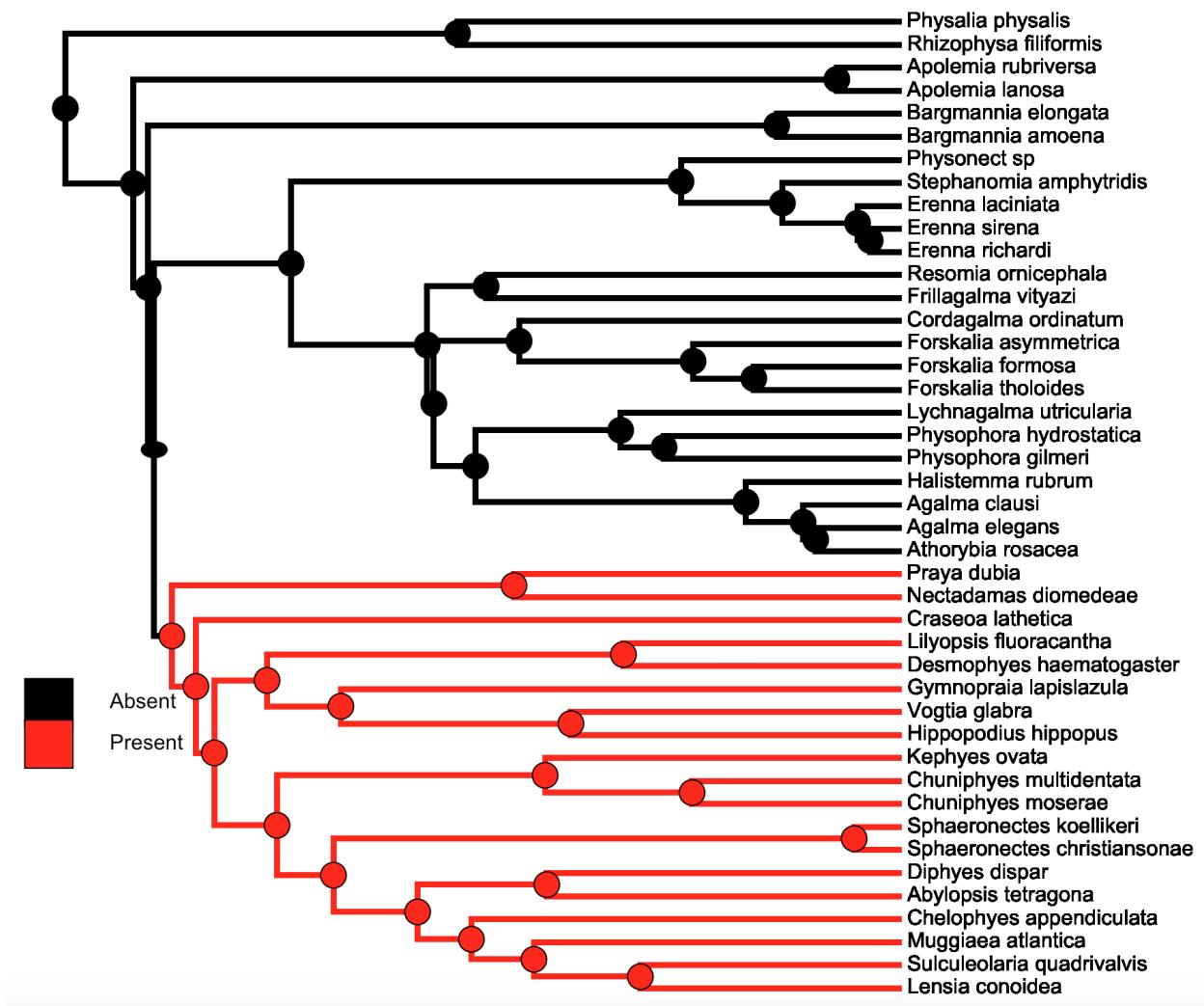


Figure 6: SIMMAP Cnidoband distal desmonemes presence/absence.

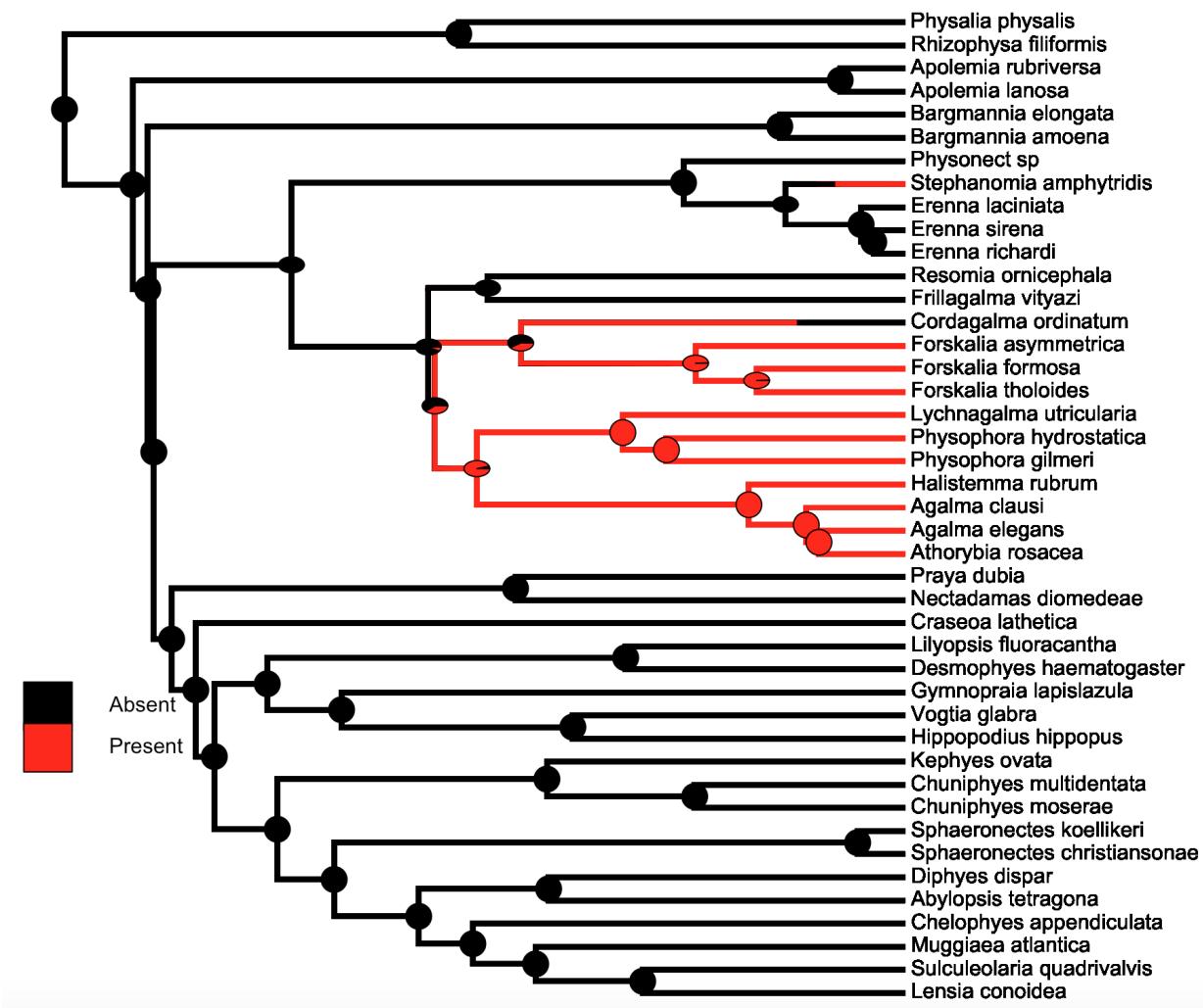


Figure 7: SIMMAP Coiled cnidoaband phenotype presence/absence.

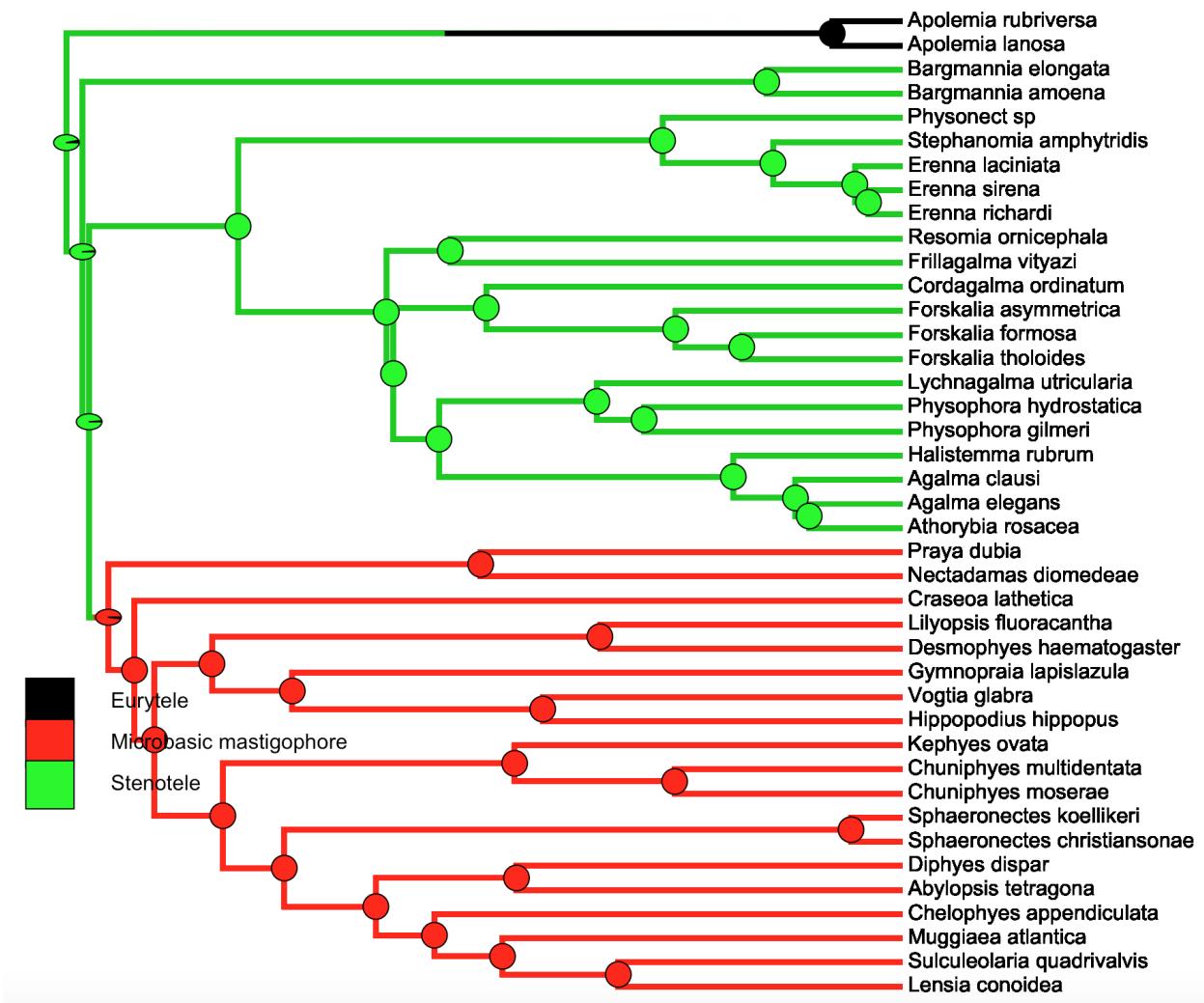


Figure 8: SIMMAP Heteroneme type.

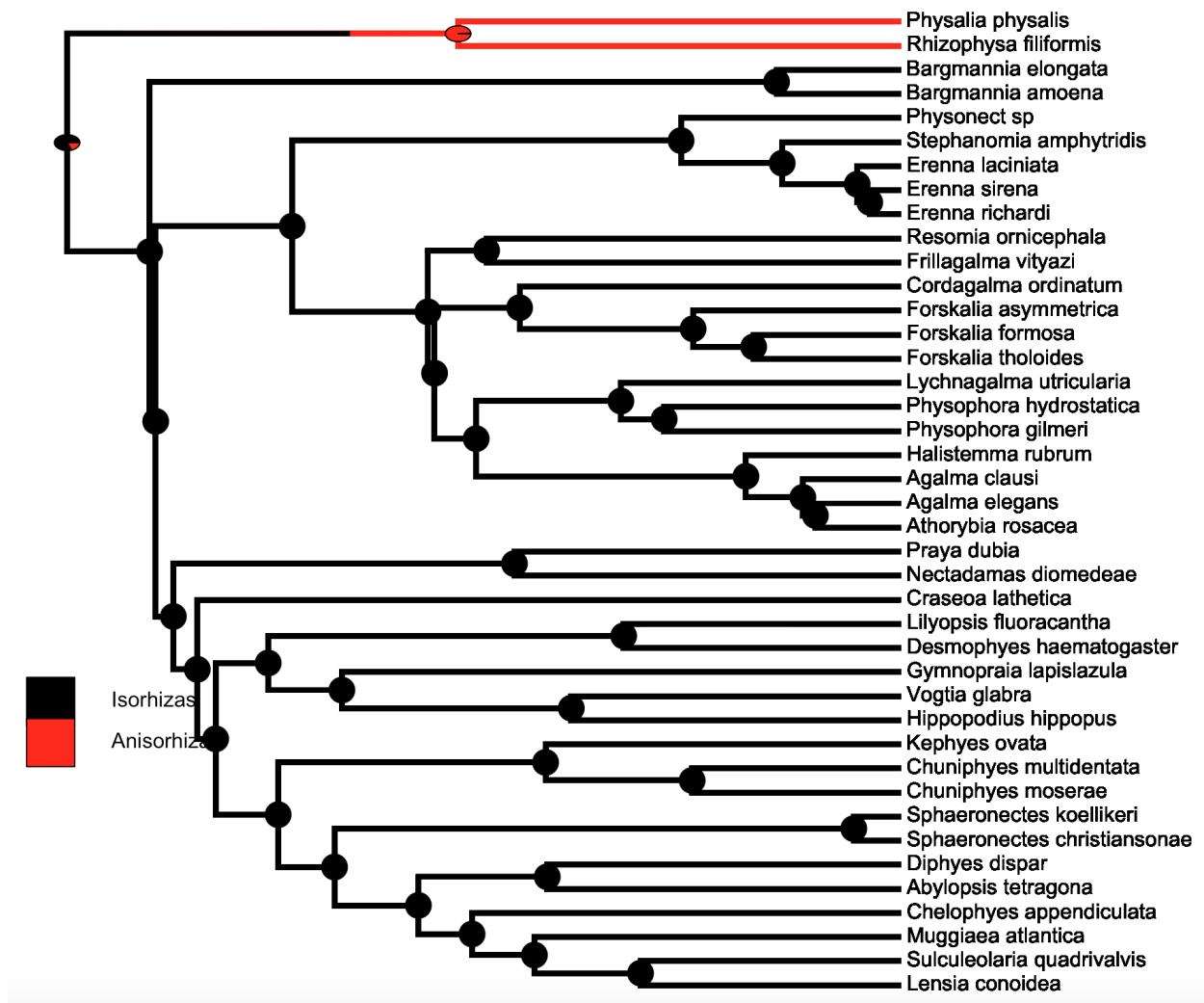


Figure 9: SIMMAP Haploneeme type.

Character	Non-Phylogenetic dAIC	BM dAIC	EB dAIC	OU dAIC	K	K p-value	Ntaxa
Haploneme elongation	0	2.017	4.332	2.38	0.583	0.001	43
Desmoneme elongation	0	3.232	5.693	3.183	0.018	0.864	31
Heteroneme shaft width $\mu\text{m}$	0	5.346	7.67	2.581	0.45	0.005	42
Elastic strand width $\mu\text{m}$	0	1526	3.938	1.296	0.706	0.001	34
Desmoneme length $\mu\text{m}$	0.518	0	2.46	0.578	0.566	0.002	31
Heteroneme shaft extension	0.589	0	2.324	1.965	0.041	0.970	42
Haploneme SA/V	0.91	0	2.315	2.291	0.156	0.132	43
Total heteroneme volume $\mu\text{m}^3$	0.961	0	2.352	2.328	0.248	0.046	39
Rhopaloneme width $\mu\text{m}$	1.205	0	2.46	1.321	0.308	0.123	31
Heteroneme volume $\mu\text{m}^3$	2.002	0	2.153	2.324	0.196	0.117	42
Involucrum length $\mu\text{m}$	2.479	0	2.498	2.492	0.529	0.001	29
Tentacle width $\mu\text{m}$	2.939	0	2.307	1.974	0.367	0.044	44
Cnidoband coiledness	3.077	0	2.315	1.786	0.174	0.043	43
Total haploneme volume $\mu\text{m}^3$	3.641	0	1.852	2.296	0.198	0.267	43
Cnidoband free length $\mu\text{m}$	3.801	0	2.132	2.315	0.325	0.007	43
Heteroneme free length $\mu\text{m}$	3.82	0	2.01	1.325	0.301	0.080	42
Rhopaloneme elongation	3.852	0	2.145	2.46	0.062	0.827	31
Desmoneme width $\mu\text{m}$	3.96	0	2.46	2.121	0.553	0.004	31
Cnidoband length $\mu\text{m}$	4.094	0	1.911	2.315	0.321	0.015	43
Heteroneme number	4.262	0	2.352	2.219	0.866	0.001	39
Heteroneme shaft free length $\mu\text{m}$	4.553	0	2.324	2.321	0.331	0.126	42
Rhopaloneme length $\mu\text{m}$	5.599	0	2.46	2.457	0.589	0.001	31
Heteroneme/Cnidoband length	5.671	0	1.862	2.342	1.068	0.001	42
Pedicle width $\mu\text{m}$	6.566	0	2.253	2.315	0.541	0.001	43
Haploneme width $\mu\text{m}$	7.495	0	2.218	2.304	0.553	0.001	43
Heteroneme width $\mu\text{m}$	7.53	0	2.324	1.647	0.502	0.001	42
Heteroneme elongation	14.169	0	0.819	2.23	0.508	0.001	42
Haploneme row number	19.566	0	2.114	2.315	0.442	0.001	43
Total nematocyst volume $\mu\text{m}^3$	21.007	0	2.213	2.292	1.3	0.001	45
Cnidoband width $\mu\text{m}$	5.69	0.307	0	2.623	0.374	0.001	43
Haploneme free length $\mu\text{m}$	12.337	7.125	0	9.439	1.079	0.001	43

Non-phylogenetic model supported

Brownian Motion model supported

Early Burst model supported

Figure 10: Model support (delta AICc), phylogenetic signal (Blomberg's K), and phylogenetic signal permutation test p-value for each continuous character. Ntaxa = Number of taxa used in the analyses after removing those where the character state is inapplicable or the data is missing.

Variable	Best model	Msig	Cvar	Svar	Sasr	Shgt	Dcfid
Desmoneme length $\mu\text{m}$	WN	0.889	0.224	0.084	0.32	0.146	0
Heteroneme shaft extension	WN	0.861	0	0.577	0	0.533	0.042
Total heteroneme volume	WN	0.895	0.577	0.006	0.026	0.078	0.603
Rhopaloneme width $\mu\text{m}$	WN	0.823	0.42	0.182	0.014	0.531	0.006
Haploneme free length $\mu\text{m}$	EB	0.841	0.052	0.036	0.168	0.226	0.843
Heteroneme volume $\mu\text{m}^3$	BM	0.855	0.731	0.228	0.897	0.775	0.104
Involucrum length $\mu\text{m}$	BM	0.839	0.01	0.018	0.116	0.09	0.987
Tentacle width $\mu\text{m}$	BM	0.817	0.841	0.402	0.386	0.785	0.48
Cnidoband coiledness	BM	0.873	0	0.028	0.016	0.144	0.41
Total haploneme volume	BM	0.807	0.228	0.004	0.006	0.024	0.398
Cnidoband free length $\mu\text{m}$	BM	0.825	0.076	0.002	0	0.006	0.681
Heteroneme free length $\mu\text{m}$	BM	0.859	0.392	0.386	0.056	0.591	0.284
Rhopaloneme elongation	BM	0.873	0.022	0.006	0.004	0.048	0.104
Desmoneme width $\mu\text{m}$	BM	0.813	0.877	0.531	0.014	0.941	0.014
Cnidoband length $\mu\text{m}$	BM	0.829	0.096	0	0	0.004	0.901
Heteroneme number	BM	0.823	0.312	0	0.004	0.02	0.869
Heteroneme shaft free length $\mu\text{m}$	BM	0.877	0.468	0.565	0.034	0.841	0.851
Rhopaloneme length $\mu\text{m}$	BM	0.829	0.525	0.547	0.01	0.917	0.08
Heteroneme/cnidoband length	BM	0.839	0.01	0	0.004	0.008	0.715
Cnidoband width $\mu\text{m}$	BM	0.907	0.977	0	0.002	0.01	0.11
Pedicle width $\mu\text{m}$	BM	0.817	0.931	0.476	0.088	0.969	0.813
Haploneme width $\mu\text{m}$	BM	0.881	0.805	0.12	0.294	0.511	0.15
Heteroneme width $\mu\text{m}$	BM	0.849	0.142	0.156	0.356	0.819	0.278
Heteroneme elongation	BM	0.933	0.094	0.07	0.681	0.791	0.777
Haploneme row number	BM	0.863	0	0.002	0.004	0.008	0.012
Total nematocyst volume	BM	0.809	0.521	0.024	0.016	0.198	0.837
Haploneme surface: volume	BM	0.831	0.945	0.130	0.503	0.426	0.170

Figure 11: P-values of the model adequacy score tests for the best model supported for each morphological character. Cvar = coefficient of variation of the absolute value of the contrasts. Svar = Slope of a linear model fitted to the absolute value of the contrasts against their expected variances. Sasr = slope of the contrasts against the ancestral state inferred at each corresponding node. Shgt = slope of the contrasts against node depth. Dcfid = Kolmogorov-Smirnov D-statistic comparing contrasts to a normal distribution with SD equal to the root of the mean of squared contrasts. P-values  $< 0.05$  were highlighted in grey, indicating significant deviations between the model and the observed data.

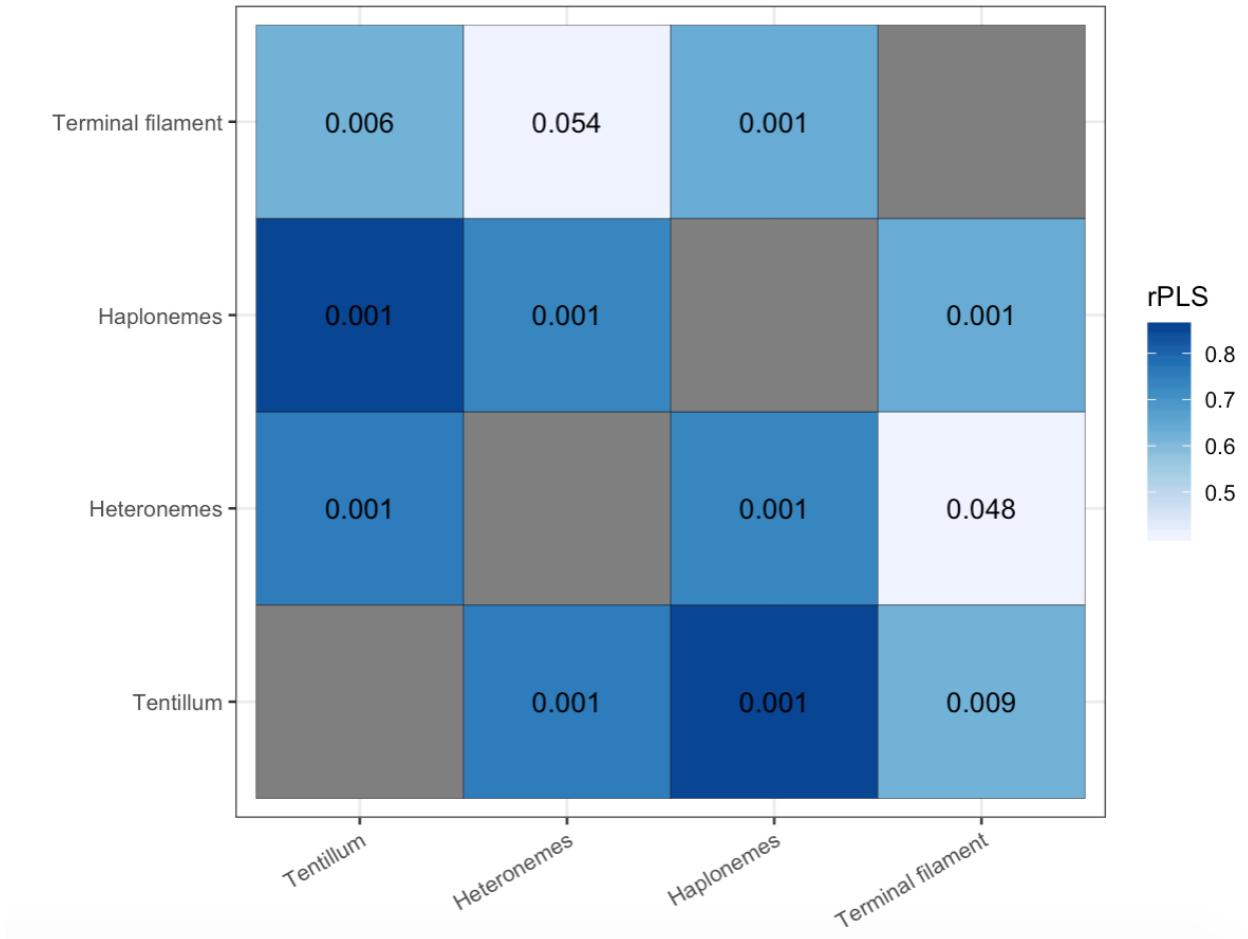
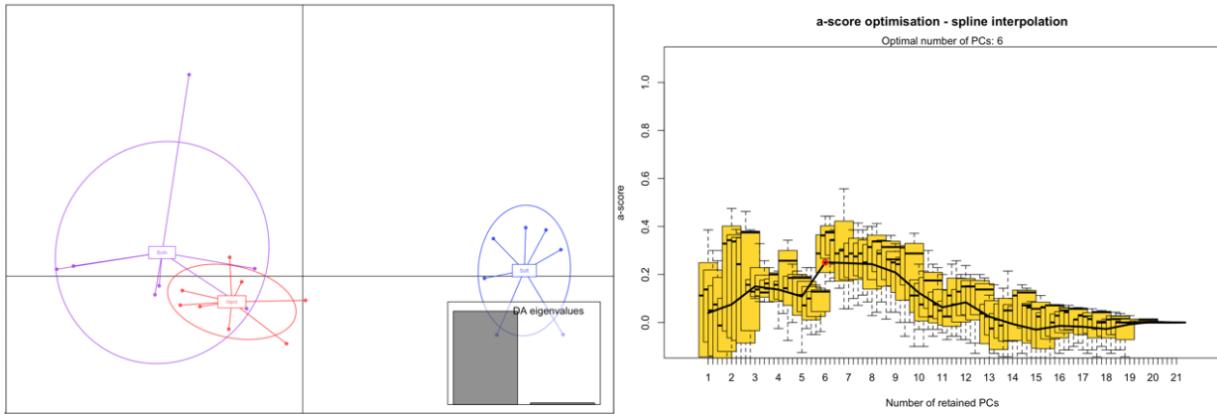


Figure 12: Heatmap showing the phenotypic integration between character modules accounting for phylogeny. Text in cells shows p-values. Color indicates the partial least squares (PLS) multivariate correlation coefficients.



### Variable contribution

Involucrum.length..um.	24.425696
Heteroneme.number	18.129947
Heteroneme.volume..um3.	6.849738
Tentacle.width..um.	6.587487
Total_nematocyst_volume	5.606488
total_haploneme_volume	4.185115
Elastic.strand.width..um.	3.584917
Heteroneme.free.length..um.	3.014292

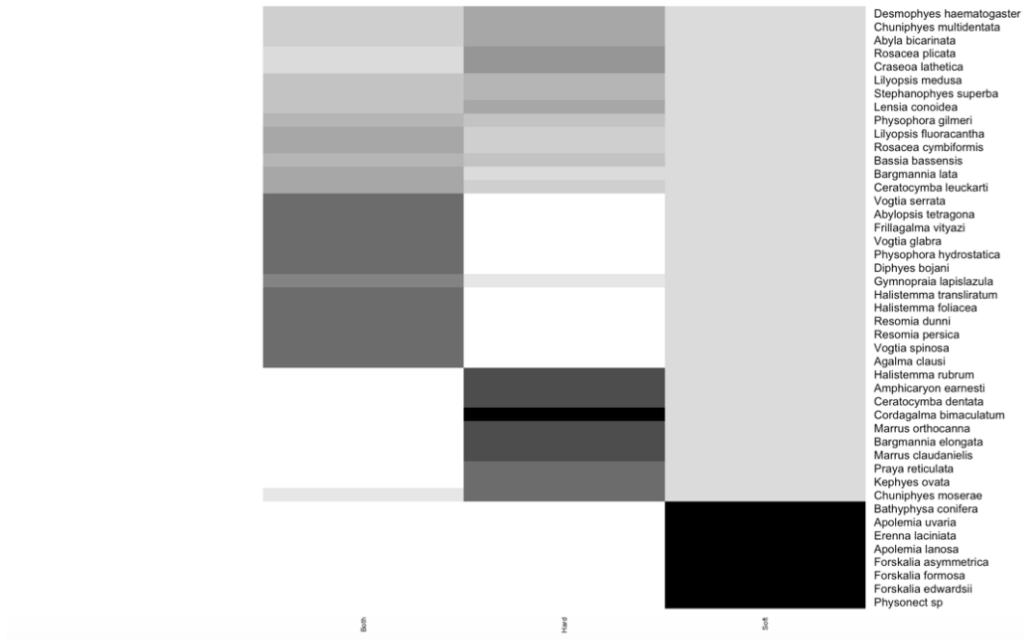


Figure 13: DAPC for soft-bodied vs. hard bodied prey specialization. Six PCs retained after a-score optimization (100 iterations). Two LDA functions used. Discriminant power on training set: 90.9%. Grayscale heat map shows the posterior probability distribution of the predictions. Variable contribution (top quartile) calculated by the sum of the LDA variable loadings weighted by the eigenvalue of each LDA.

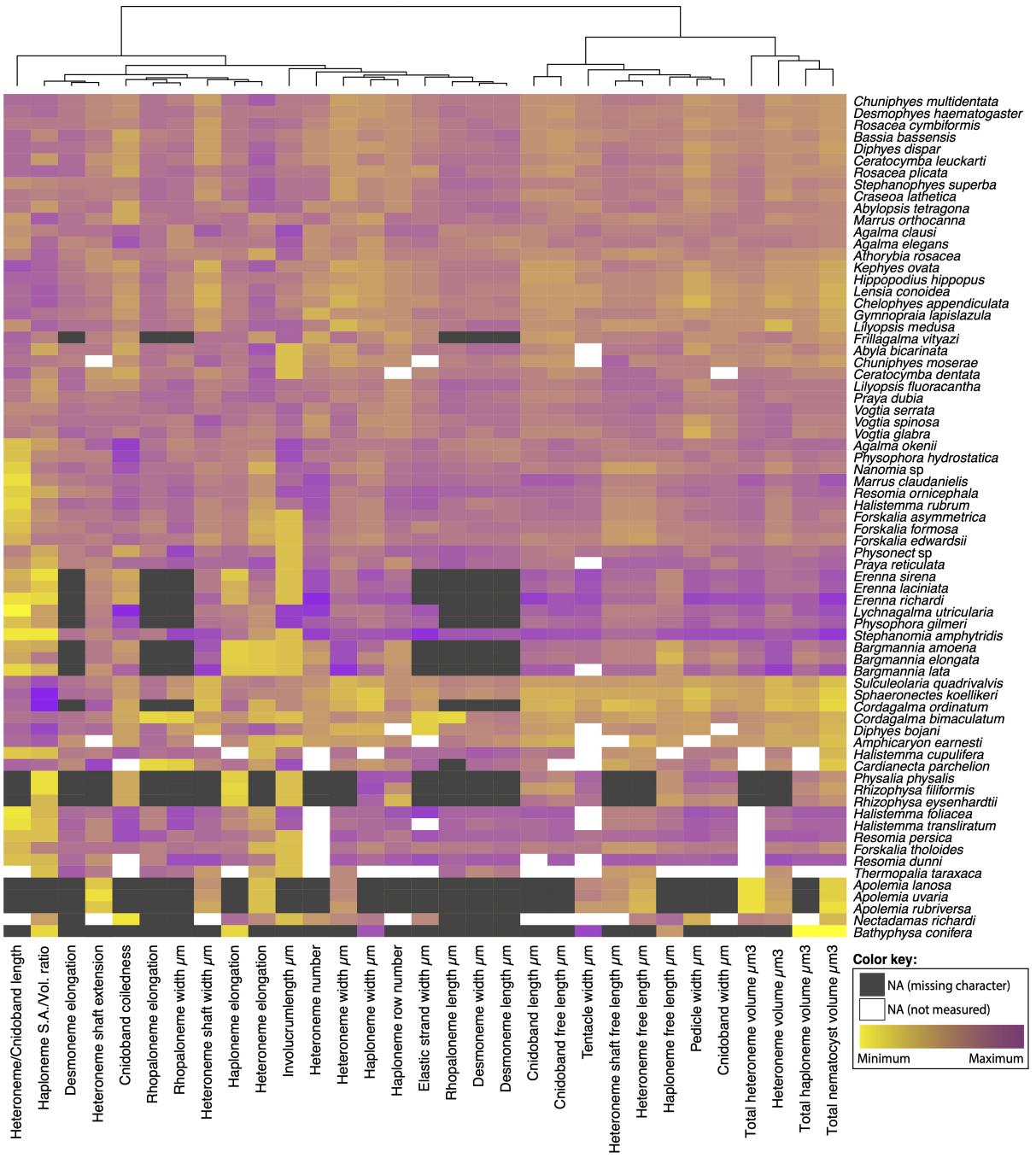


Figure 14: Heatmap summarizing the morphological diversity measured in Damian-Serrano *et al.* 2020 for 96 species of siphonophores clustered by similarity (raw data published in Damian-Serrano 2020). Missing values from absent characters presented as dark grey cells, missing values produced from technical difficulties presented as white cells. Values scaled by character.

**S1.1) Definitions of homologous structures used throughout this work.**

Structure	Definition
Haploneme	Nematocyst with no shaft
Heteroneme	Nematocyst with a distinct shaft
Desmoneme	Small oval/tapered adhesive nematocyst with thick coiled tubule
Rhopaloneme	Small rod-like nematocyst found on the terminal filament
Terminal filament	Distal extension of the tentillum beyond the cnidoband
Cnidoband	Distinct packing of nematocysts on the dorsal side of the tentillum
Tentacle	Tubular projection from the gastrozooid basigaster
Tentillum	Evenly spaced dorsal evagination of the tentacle carrying ordered and functional nematocysts
Involucrum	Extension of the pedicle covering part of the cnidoband
Pedicle	Proximal region of the tentillum between the cnidoband and the tentacle
Elastic strand	Mesoglea derived collagenous double strand underlying the cnidoband of some siphonophores

**S1.2) Definitions of the continuous morphological and kinematic characters measured.**

Character	Definition	Units
Cnidoband length	Distance from the base to the tip of the cnidoband in natural position	micrometers
Cnidoband free length	Distance from the base to the tip of the cnidoband when stretched straight	micrometers
Cnidoband width	Diameter of the cnidoband on the widest point	micrometers
Involucrum length	Length of the involucrum from the base of the cnidoband to its most distal extent	micrometers
Heteroneme length	Length of the heteronemes	micrometers
Heteroneme width	Diameter of the heteronemes at the widest point	micrometers
Heteroneme shaft length	Length of the heteroneme shaft	micrometers
Heteroneme shaft width	Width of the heteroneme shaft	micrometers
Heteroneme number	Number of heteronemes in each tentillum (# in each row*2)	micrometers
Haploneme length	Length of the haplonemes	micrometers
Haploneme width	Diameter of the haplonemes at the widest point	micrometers
Rhopaloneme length	Length of the rhopalonemes	micrometers
Rhopaloneme width	Diameter of the rhopalonemes at the widest point	micrometers
Desmoneme length	Length of the desmonemes	micrometers
Desmoneme width	Diameter of the cnidoband at the widest point	micrometers
Involucrum length	Length of the involucrum from the base of the cnidoband to its most distal extent	micrometers
Elastic strand width	Diameter of the descending elastic strand at the widest point	micrometers
Pedicle width	Diameter of the pedicle	micrometers
Tentacle width	Diameter of the tentacle	micrometers
Haploneme row number	Number of haploneme rows running parallel to the length of the cnidoband	micrometers
Cnidoband coiledness	Cnidoband free length / Cnidoband length	adimensional
Heteroneme elongation	Heteroneme Length/Width	adimensional
Haploneme elongation	Haploneme Length/Width	adimensional
Desmoneme elongation	Desmoneme Length/Width	adimensional
Rhopaloneme elongation	Rhopaloneme Length/Width	adimensional
Heteroneme shaft extension	Heteroneme shaft length / Heteroneme capsule length	adimensional
Nematocyst Surface area	$4\pi r^2 \left( ((Length/2)^2 * (Width/2)^2)^{1.6} + (((Width/2)^2)^2 * 1.6) / 3 \right)^{1/1.6}$	micrometers squared
Nematocyst volume	Ellipsoid formula : $(4/3)\pi r^3 (Length/2)^2 * (Width/2)^2$	micrometers cubed
Nematocyst SA/V ratio	Nematocyst surface area / Nematocyst volume	1/micrometers
Total haploneme volume	Haploneme volume * Haploneme row number * (Cnidoband free length / Haploneme width)	micrometers cubed
Total heteroneme volume	Heteroneme volume * Heteroneme number	micrometers cubed
Total nematocyst volume	Total haploneme volume + Total heteroneme volume	micrometers cubed

Figure 15: Character definitions.

1) Microscope slides and specimens measured. Catalog numbers correspond to accessions in the Yale Peabody Museum of Natural History, Invertebrate Zoology collection.

Slide_ID	Species	Specimen	Accession number	Catalog number
S2	<i>Abyla bicarinata</i>	BWP 2053-13	YPM.12903	TBD
M2	<i>Abylopsis tetragona</i>	VFSS 13-04-11	YPM.12903	TBD
R9	<i>Abylopsis tetragona</i>	VF#15	YPM.12903	TBD
T6	<i>Abylopsis tetragona</i>	SL0303S	YPM.12903	TBD
U6	<i>Abylopsis tetragona</i>	JSL I 2950-CG-7	YPM.12903	TBD
V6	<i>Abylopsis tetragona</i>	JSL I 2953-CG-3	YPM.12903	TBD
V4	<i>Agalma clausi</i>	BWP 1092-6	YPM.12903	TBD
H6	<i>Agalma elegans</i>	VF2016-5	YPM.12903	TBD
I6	<i>Agalma elegans</i>	SL0210	YPM.12903	TBD
I9	<i>Agalma elegans</i>	RI3-7-18	YPM.12903	TBD
J6	<i>Agalma elegans</i>	BWD100212MB	YPM.12903	TBD
Q2	<i>Agalma elegans</i>	SL0205T	YPM.12903	TBD
B9	<i>Agalma okenii</i>	BWP 786-19	YPM.12903	TBD
C9	<i>Agalma okenii</i>	BWP 792-36	YPM.12903	TBD
D9	<i>Agalma okenii</i>	D724-BW3-3	YPM.12903	TBD
H9	<i>Agalma okenii</i>	D723-BW3-1	YPM.12903	TBD
O1	<i>Agalma okenii</i>	BWP 565-5	YPM.12903	TBD
P2	<i>Amphicaryon earnesti</i>	Discovery St. 7856#24	YPM.12903	TBD
B11	<i>Apolemia lanosa</i>	D1024-D1	YPM.12738	TBD
M3	<i>Apolemia lanosa</i>	D858-D6	YPM.12903	TBD
O7	<i>Apolemia lanosa</i>	D614-D2	YPM.12903	TBD
P7	<i>Apolemia lanosa</i>	D668-SS1	YPM.12903	TBD
Q7	<i>Apolemia lanosa</i>	D552-SS8	YPM.12903	TBD
A9	<i>Apolemia rubriversa</i>	D558-D4	YPM.12903	TBD
D8	<i>Apolemia rubriversa</i>	D651-D5	YPM.12903	TBD
H10	<i>Apolemia rubriversa</i>	D551-D5	YPM.12903	TBD
O10	<i>Apolemia rubriversa</i>	T673-D2	YPM.12903	TBD
Q3	<i>Apolemia rubriversa</i>	D668-D7	YPM.12903	TBD

Figure 16: Specimen catalog.