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1 On the Origin of Oxygenic Photosynthesis and Cyanobacteria

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23 Photosystem I, Photosystem II, Proterozoic, water oxidation

24

25 **Summary**

26 Oxygenic phototrophs have played a fundamental role in Earth's history by enabling the rise
27 of atmospheric oxygen (O₂) and paving the way for animal evolution. Understanding the origin
28 of oxygenic photosynthesis and Cyanobacteria are key when piecing together the events around
29 Earth's oxygenation. It is likely that photosynthesis evolved within bacterial lineages that are
30 not extant, so it can be challenging when studying the early history of photosynthesis. Recent
31 genomic and molecular evolution studies have transformed our understanding about the
32 evolution of photosynthetic reaction centres and the evolution of Cyanobacteria. The evidence
33 reviewed here highlights some of the most recent advances on the origin of photosynthesis both
34 at the genomic and gene family level.

35

36 **Introduction**

37

38 **I. What is the evidence for the origin of oxygenic photosynthesis and** 39 **Cyanobacteria?**

40

41 Oxygenic photosynthesis is one of the most important metabolisms to have evolved on Earth
42 as it enabled complex life to emerge. A fundamental question in biology is when oxygenic
43 photosynthesis first evolved. It underpinned both biological and geological processes that led
44 to the rise of O₂ during the Early Earth. Regarding the timing of origin, the fossil record of
45 Cyanobacteria is not conclusive (Schirromeister *et al.*, 2016). Similar fossil evidence has shown
46 that molecular biomarkers are no longer reliable (Rasmussen *et al.*, 2008).

47

48 Different lines of geochemical evidence have constrained the major oxygenation events
49 observed during Early Earth. The first rise of oxygen in the atmosphere, known as the Great
50 Oxidation Event (GOE) ~ 2.32-2.4 Billion years ago (Bya) (Bekker *et al.*, 2004; Lyons *et al.*,
51 2014), has been well constrained based on geochemical proxies (Lyons *et al.*, 2014). The GOE
52 represents the minimum age for the origin of oxygenic photosynthesis and the emergence and
53 diversification of oxygen-requiring metabolic and biosynthetic pathways (Raymond & Segre,
54 2006). A second major oxygenation event known as the Neoproterozoic Oxidation Event
55 (NOE) ~800-600 Million years ago (Mya), significantly increased atmospheric O₂
56 concentrations (Scott *et al.*, 2008) similar to those found in today's atmosphere. The NOE has

57 also been linked to the origin of animals, major glaciation events and huge disruptions to the
58 carbon cycle (Lyons *et al.*, 2014), and more recently to the emergence of marine planktonic
59 groups (Brocks *et al.*, 2017). Over geological time, O₂ in our atmosphere has accumulated
60 because carbon fixation by oxygenic phototrophs has exceeded respiration of organic matter.
61 Simultaneously, the imbalance of these two processes has resulted in the drawdown of carbon
62 and burial of organic carbon in marine sediments (Holland, 2006).

63 While it is well recognised that O₂ has been the result of biological activity contributing to the
64 oxidation events during the Precambrian (Lyons *et al.*, 2014), less is known about the
65 evolutionary history of oxygenic phototrophs. How did their origination and subsequent
66 diversification into different functional groups and/or taxa contribute to shaping geological
67 processes? Clues about the evolution of early oxygenic phototrophs have been recorded in
68 their genomes, and their history can be elucidated through phylogenetic comparison and
69 comparative genomics. The evidence reviewed here focuses on the biological evidence, partly
70 because over the last decade, the increased number of genomic studies have transformed our
71 understanding on the evolution of photosynthesis and oxygenic phototrophs (Blank & Sánchez-
72 Baracaldo, 2010; Soo *et al.*, 2014; Sánchez-Baracaldo *et al.*, 2017).

73

74 **II. Timing of divergence of oxygenic photosynthesis and major** 75 **Cyanobacteria groups**

76 Genomics and evolutionary studies have provided insights into the evolution of core proteins
77 involved in oxygenic photosynthesis (Cardona, 2018; Cardona *et al.*, 2019) and the appearance
78 of Cyanobacteria's common ancestor (Blank & Sánchez-Baracaldo, 2010; Schirrmeyer *et al.*,
79 2013; Shih *et al.*, 2016). Amongst prokaryotes, Cyanobacteria have some of the best fossil
80 records (Schirrmeyer *et al.*, 2016) enabling molecular clock studies. Ages estimates of the
81 gene family of PSI and PSII (Cardona, 2018; Cardona *et al.*, 2019) are consistent with
82 geological records showing traces of oxygen throughout the Archean (4–2.5 Bya); these
83 findings imply that oxygenic photosynthesis was already established by 3.0 Bya *et al.*, 2014;
84 Wang *et al.*, 2018). In other words, early forms of water oxidation, carried out by ancestral
85 homodimeric photosystems (Figures 1 and 2), could have originated a billion years before the
86 GOE (Cardona *et al.*, 2019). Furthermore, the standard heterodimeric photosystems, a defining
87 trait of crown group Cyanobacteria (Figure 3), evolved towards the late Archean (Blank &

88 Sánchez-Baracaldo, 2010; Schirromeister *et al.*, 2015) or early Paleoproterozoic (Shih *et al.*,
89 2016).

90 The majority of extant Cyanobacterial diversity evolved after the GOE (Figure 3) (Sánchez-
91 Baracaldo, 2015). For instance, the closest relatives (i.e., *Gloeomargarita*) of the
92 Archaeplastida, a monophyletic group that includes the glaucophytes, red algae, the green algae
93 and land plants emerged ~1.9 billion years ago (Sánchez-Baracaldo *et al.*, 2017). In more
94 recent time scales, the age estimation of marine planktonic groups is consistent with
95 geochemical evidence supporting the timing of the ocean oxygenation at around 800–600 Mya
96 (Sánchez-Baracaldo *et al.*, 2014). Age estimates of marine green algae (Sánchez-Baracaldo *et*
97 *al.*, 2017) at the end of the Precambrian and prior to the origin of animals are consistent with
98 eukaryote biomarker data (Brocks *et al.*, 2017). Molecular clock studies of symbiotic
99 associations have also shown that age estimates of the symbiont, UCYN-A, overlap with fossil
100 ages of its host, *Braarudosphaera bigelowii*, at around 92 Mya (Cornejo-Castillo *et al.*, 2016).

101

102 **III. The origin of Photosystem II (PSII) vs the origin of Cyanobacteria**

103 Photosynthesis is an ancient metabolism that likely evolved in lineages that are no longer
104 extant. Today photosynthetic reaction centres are found amongst at least eight extant bacterial
105 lineages: Cyanobacteria, Proteobacteria, Chloroflexi, Acidobacteria, Chlorobi, Firmicutes,
106 Gemmatimonadetes, and the newly discovered Candidatus Eremiobacterota (Figure 1) (Hug *et*
107 *al.*, 2016; Ward *et al.*, 2019). Since oxygenic photosynthesis is only found in Cyanobacteria,
108 and other groups of bacteria evolved different types of anoxygenic photosynthesis (Hohmann-
109 Marriott & Blankenship, 2011), it is often assumed that the appearance of oxygenic
110 photosynthesis coincided with the origin of Cyanobacteria (Soo *et al.*, 2017). While to an
111 extent, it is reasonable to interchange both terms, there are significant differences when
112 referring to oxygenic photosynthesis and Cyanobacteria. At the gene family level, the origin
113 of reaction centre proteins elucidate the origin of photosynthetic water oxidation (Cardona,
114 2018; Cardona *et al.*, 2019). At the organismal level, phylogenomic approaches unravel the
115 evolutionary history of organisms that are currently able to perform oxygenic photosynthesis
116 (Blank & Sánchez-Baracaldo, 2010; Schirromeister *et al.*, 2013; Schirromeister *et al.*, 2016).
117 Both approaches have helped piece together biological events that have been obscured by over
118 3 billion years of history.

119 It has been widely assumed that oxygenic photosynthesis emerged from ancestral anoxygenic
120 phototrophs (Hohmann-Marriott & Blankenship 2011). Cyanobacteria have two photosystems
121 (PSI and PSII), and anoxygenic phototrophs have either PSI or PSII-like photosystems. Some
122 have proposed that a “protocyanobacteria” containing two anoxygenic photosystems predated
123 Cyanobacteria from an ancient duplication (Mulkidjanian *et al.*, 2006; Martin *et al.*, 2018),
124 whereas others have put more emphasis on whether the photosystems emerged by horizontal
125 gene transfers (Raymond *et al.*, 2002). Recent work bringing together comparative structural
126 biology and phylogenetic analyses have challenged some of these older perspectives. It is now
127 argued that the photosystems (marked 1 in Figure 1) uniquely evolved the ability to perform
128 water oxidation from the beginning, and as the photosystems further specialised, it led to what
129 we now know as oxygenic photosynthesis (Cardona, 2017; Cardona, 2019; Cardona &
130 Rutherford, 2019). It is worth highlighting that the efficiency of enzymes carrying out water
131 oxidation has changed and improved, and earlier forms predate the evolution of crown group
132 Cyanobacteria (Cardona *et al.*, 2019) (marked 5 in Figure 1, and Figure 3).

133 Large scale phylogenetic analyses have confirmed that photosynthetic organisms are
134 polyphyletic, or do not share a recent common ancestor (Cardona, 2015; Hug *et al.*, 2016). In
135 other words, lineages of phototrophs are often closely related to non-photosynthetic lineages.
136 This is the case for Cyanobacteria, in which their sister groups are non-photosynthetic such as
137 the Melainabacteria (Di Rienzi *et al.*, 2013), and the Sericytochromatia (Soo *et al.*, 2017).
138 Melainabacteria and Sericytochromatia lack genes involved in photosynthesis (Soo *et al.*,
139 2017) and likely lost the ability to perform photosynthesis after their divergence from
140 Cyanobacteria. Phylogenetic and comparative analyses further indicate that the most recent
141 common ancestor of Cyanobacteria was already a highly sophisticated phototroph capable of
142 water oxidation (Blank & Sánchez-Baracaldo, 2010; Cardona *et al.*, 2015).

143

144 **IV. PSII**

145 The core of cyanobacterial PSII consists of D1 and D2 (Figure 2), which originated from an
146 ancient gene duplication event (marked 4 in Figure 1). These proteins are associated with two
147 core antenna subunits named CP43 and CP47 (Figure 2), which also originated from an ancient
148 gene duplication event. The origin of water oxidation likely predated these two duplication
149 events (Rutherford & Faller, 2003; Cardona *et al.*, 2019). Biochemical evidence implies that

150 the ancestral homodimeric PSII (marked 4 in Figure 1) was a highly-oxidising, oxygen-
151 producing photosystem that had already evolved the capacity to protect against the formation
152 of reactive oxygen species (Cardona *et al.*, 2019).

153 In-depth analysis of the rates of evolution of PSII suggest that the gene duplication associated
154 with evolution of D1 and D2 (marked 4 in Figure 1) predated the most recent common ancestor
155 of Cyanobacteria (marked 5 in Figure 1) (Cardona *et al.*, 2019). PSII is the slowest evolving
156 photosystem, displaying rates of evolution up to five times slower than those of anoxygenic
157 photosystems. This means that the earliest Type II reaction centres (marked 2 in Figure 1),
158 previously thought to be similar to those present in purple bacteria (Proteobacteria, marked 6
159 in Figure 1), were more like cyanobacterial PSII. When comparing the overall structural
160 architecture of the photosystems (Figure 2), it emerges that cyanobacterial PSII retains a greater
161 number of ancestral traits than the reaction centres of Proteobacteria and Chloroflexi (Cardona
162 & Rutherford 2019). It is worth highlighting that the deep divergence of anoxygenic and
163 oxygenic photosystems (marked 2 and 3 in Figure 1), could have been a response to dealing
164 with oxygen itself (Orf *et al.*, 2018; Cardona, 2019). In other words, the origin of water
165 oxidation to oxygen not only predated the D1 and D2 duplication (marked 4 in Figure 1), but
166 may have coincided with the emergence of the two distinct families of reaction centres
167 themselves (marked 1 in Figure 1) (Cardona & Rutherford, 2019).

168

169 **V. Crown group Cyanobacteria**

170 Within prokaryotic groups, Cyanobacteria are one of the most morphologically diverse -
171 growth forms range from unicellular to filamentous or multicellular (Castenholz, 2001; Shih *et al.*
172 *et al.*, 2013). Not long ago, most of the available genome data for Cyanobacteria were biased
173 toward marine unicellular taxa (e.g., *Synechococcus* and *Prochlorococcus*) (Shih *et al.*, 2013).
174 Within the last five years, a number of studies have isolated and sequenced lineages covering
175 a wider range of taxonomic diversity and habitats within the tree of life of Cyanobacteria.
176 Some of these studies have included: *Gloeomargarita* also known as the closest known relative
177 of the chloroplast (Ponce-Toledo *et al.*, 2017; Sánchez-Baracaldo *et al.*, 2017); *Pseudanabaena*
178 (Schirromeister *et al.*, 2015b); symbiotic groups from both marine and freshwater habitats (e.g.,
179 UCYN-A, *Richelia*, *Epithemia*, *Rhopalodia*) (Hilton *et al.*, 2013; Bombar *et al.*, 2014;
180 Nakayama *et al.*, 2014; Cornejo-Castillo *et al.*, 2016); extremophiles from cold extreme
181 habitats (Christmas *et al.*, 2016; Christmas *et al.*, 2018); underrepresented freshwater genomes

182 (Di Cesare *et al.*, 2018; Sánchez-Baracaldo *et al.*, 2019); and genomes from continental
183 subsurfaces (Puente-Sánchez *et al.*, 2018).

184 The availability of new genomes and large-scale phylogenetic analyses have helped resolve
185 deep-branching relationships within Cyanobacteria, providing insights into the evolution of
186 morphology and habitat within this Phylum (Blank & Sánchez-Baracaldo, 2010; Shih *et al.*,
187 2013; Schirrmeyer *et al.*, 2015). Genomic data combined with advances in phylogenetic and
188 trait evolution analyses have filled gaps in the geological record by providing testable
189 hypotheses about the ancestral habitat of ancestral Cyanobacteria (Blank & Sánchez-
190 Baracaldo, 2010; Schirrmeyer *et al.*, 2016; Sánchez-Baracaldo *et al.*, 2017).

191 Trait evolution analyses have shown that early divergent Cyanobacteria likely inhabited low
192 salinity and terrestrial environments (Blank & Sánchez-Baracaldo, 2010). The earliest
193 Cyanobacteria forms were unicellular and had small cell diameters (*Gloeobacter*,
194 *Synechococcus*-like) (Larsson *et al.*, 2011; Sánchez-Baracaldo, 2015). Filamentous forms
195 appeared shortly afterwards and likely resembled extant *Pseudanabaena* lineages (Figure 3)
196 (Schirrmeyer *et al.*, 2011; Sánchez-Baracaldo, 2015). Their emergence would have facilitated
197 the formation of microbial mats increasing their ecological dominance during the Proterozoic
198 (Sánchez-Baracaldo, 2015; Schirrmeyer *et al.*, 2016). The origin of multicellularity in
199 Cyanobacteria was a significant biological innovation that has been previously associated with
200 increased diversification rates around the GOE (Schirrmeyer *et al.*, 2013) resulting in most of
201 the diversity of extant Cyanobacteria, including recently described groups such as
202 Macrocyanoacteria (cell diameters larger than 3 μm up to 50 μm) and Microcyanoacteria
203 (cell diameters ranging from $\sim 1\text{-}2 \mu\text{m}$) (Sánchez-Baracaldo, 2015).

204 The great majority of extant Cyanobacteria are found in terrestrial and freshwater
205 environments, and often thrive as pioneer species in habitats such as drylands, glaciers and the
206 open ocean (Castenholz, 2001; Blank & Sánchez-Baracaldo, 2010). Phylogenomic analyses
207 have further revealed that marine planktonic lineages are derived taxa (Sánchez-Baracaldo *et*
208 *al.*, 2014). Some of these lineages are sister to unicellular freshwater taxa (e.g.,
209 *Synechococcus*, and *Cyanothece*), filamentous freshwater (e.g., Nostocales) and benthic
210 marine mat formers (e.g., *Hydrocoleum*) (Sánchez-Baracaldo *et al.*, 2014; Sánchez-Baracaldo,
211 2015). In other words, marine planktonic lineages do not form a monophyletic group; this
212 phylogenetic pattern provides evidence for independent colonization events into open ocean

213 habitats at different times in history (Sánchez-Baracaldo *et al.*, 2014; Sánchez-Baracaldo,
214 2015; Cornejo-Castillo *et al.*, 2016; Sánchez-Baracaldo *et al.*, 2019).

215

216 **VI. Conclusions and Future Perspectives**

217 Recently available genomic data and advancements in evolutionary methodologies have helped
218 to resolve our understanding of the evolution of photosynthetic reaction centres and
219 Cyanobacteria. Biological evidence supports the view that early forms of oxygenic
220 photosynthesis were present throughout the Archean. Evolutionary studies of PSII imply that
221 oxygenic photosynthesis was already well established by 3.0 Bya reconciling geochemical and
222 molecular evolution evidence bases. Consequently, crown group Cyanobacteria may have
223 become the dominant primary producers near the late Archean as oxygenic photosynthesis
224 reached a higher level of complexity and sophistication. Most major groups of Cyanobacterial
225 diversity, including the lineage leading to chloroplasts, appeared after the GOE. Marine
226 planktonic groups evolved toward the end of the Precambrian when biomarker and molecular
227 clock analyses point to the first appearance of marine eukaryotic green algae prior to the
228 emergence of animals.

229 Some outstanding question remain regarding the evolution of photosynthesis. Further research
230 is required to fully determine the structural and photochemical characteristics of the earliest
231 known reaction centres and to identify the evolutionary incentives behind establishment of two
232 photosystems in series. This could be accomplished with ancestral sequence reconstruction
233 strategies. Future efforts should also continue uncovering diversity from early divergent
234 lineages. Close relatives of Cyanobacteria, such as Melainabacteria and Sericytochromatia,
235 have been identified almost entirely from metagenomic data. It is therefore important to isolate
236 and culture these lineages of non-photosynthetic close relatives to explore their metabolic and
237 physiological capabilities. Other basal lineages such as *Gloeomargarita* (Ponce-Toledo *et al.*,
238 2017), have revealed the closest known relatives of the chloroplast and helped to infer the
239 habitat of early photosynthetic eukaryotes (Sánchez-Baracaldo *et al.*, 2017). Finally, age
240 estimates could be improved by implementing calibration points, including new taxa and
241 experimentally measuring rates of cyanobacterial genome evolution across taxa.

242

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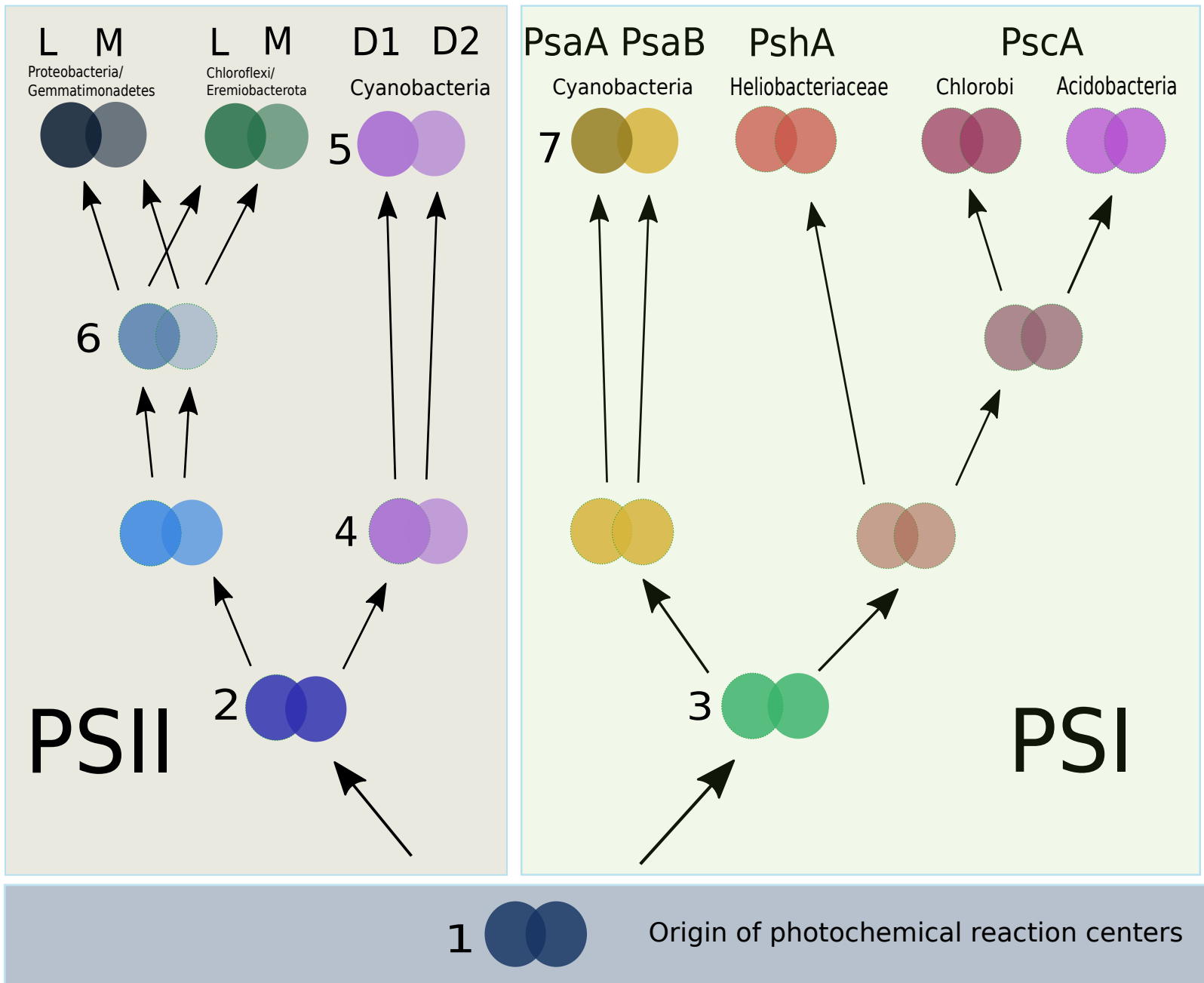
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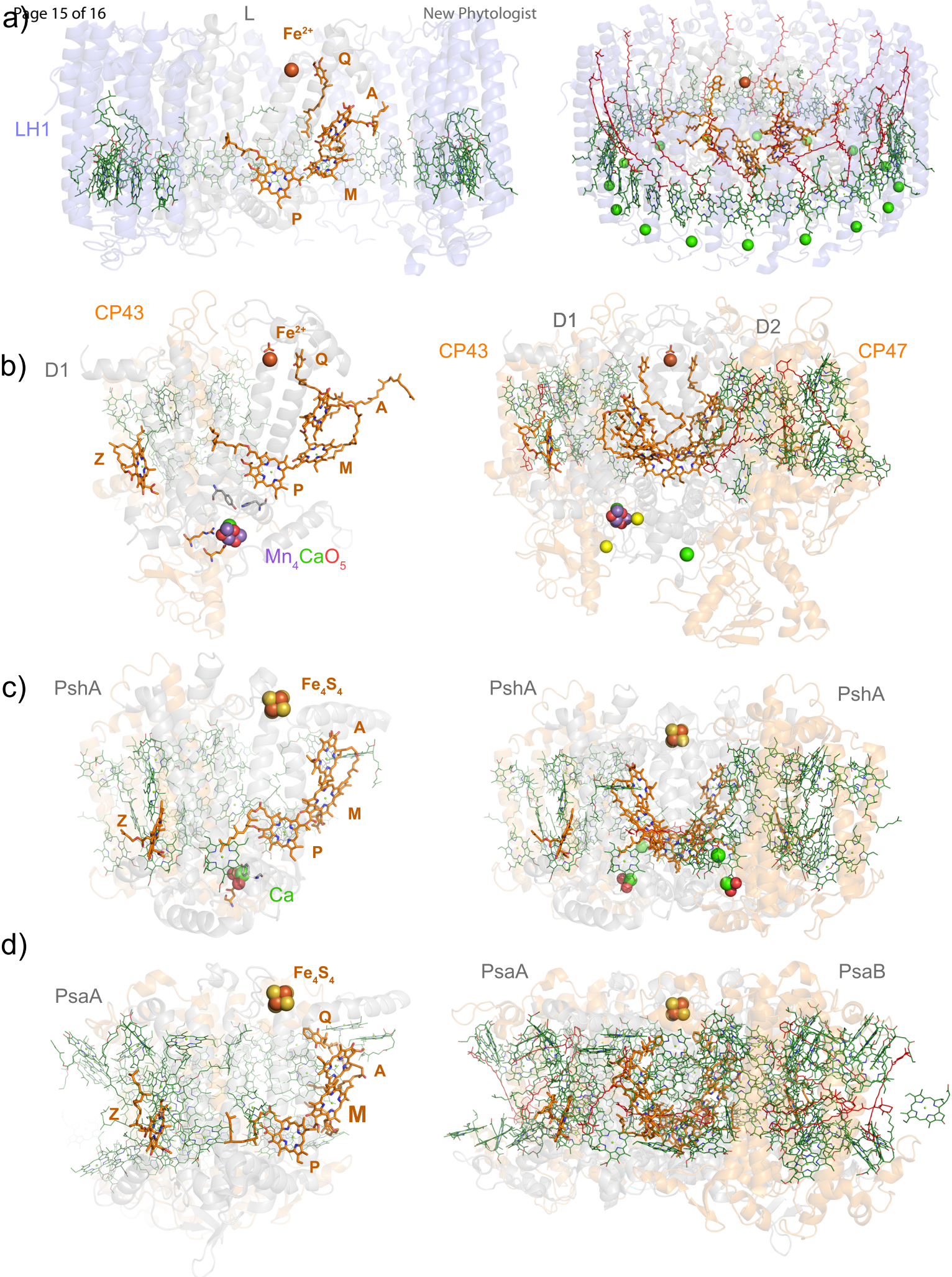
392 **Figure 1.** Schematic representation of the evolutionary relationships of reaction centre
 393 proteins based on molecular phylogenies. The ancestral photochemical reaction centre protein
 394 was likely encoded by a single gene (bottom, marked 1), which later gave rise to the first PSII-
 395 like (Type II) and PSI-like (Type I) reaction centre proteins. The monophyly of all reaction
 396 centre proteins (marked 2 and 3) implies that their origin predates the radiation of all known
 397 groups of phototrophs. At the beginning, both ancestral types were homodimeric (indicated by
 398 the same colour tone). Type II reaction centres later became heterodimeric (indicated by
 399 different colour tones) by convergent evolution in cyanobacterial PSII (marked 4) and in
 400 anoxygenic Type II reaction centres (marked 6). Crown group Cyanobacteria inherited
 401 heterodimeric PSII (marked 5) and heterodimeric PSI (marked 7).

402

403 Figure 2. Structural comparisons of anoxygenic and oxygenic photosystem cores. Monomers
 404 displaying the main redox cofactors, molecules in orange sticks, are shown in the left column
 405 and full dimeric configurations are shown in the right column. Transparent grey ribbons mark
 406 the core subunit associated with the core antenna displayed in transparent orange ribbons.
 407 Antenna (bacterio)chlorophylls are shown in green lines, with the exception of that marked as
 408 Z; carotenoids are shown in red lines. Type II reaction centres can be visually recognised by
 409 the presence of a non-heme Fe²⁺, while Type I reaction centres feature an iron-sulfur cluster,
 410 F_X. a) Anoxygenic Type II reaction centre of the purple bacteria (phototrophic
 411 Proteobacteria). Only the reaction centre core subunit L is shown surrounded by the light
 412 harvesting complex LH1 (purple ribbons). b) Oxygenic cyanobacterial PSII. The core of
 413 PSII is comprised of the reaction centre subunits D1 and D2, and the core antenna subunits
 414 CP43 and CP47. c) Homodimeric Type I reaction centre of the Heliobacteria (phototrophic
 415 Firmicutes). The core of this contains a single subunit known as PshA. d)
 416 Cyanobacterial heterodimeric PSI. The core of PSI is comprised of two subunits known as
 417 PsaA and PsaB. P (photochemical pigment), M (monomeric chlorophylls), A (primary
 418 acceptor), and Q (quinone) mark the different redox cofactors at homologous positions between
 419 different photosystems. Z denotes a core-bound antenna chlorophyll retained in PSII and Type
 420 I reaction centres but lost in the anoxygenic Type II reaction centres concomitant with the loss
 421 of core antenna and the evolution of a new light harvesting system.

422
423 **Figure 3.** Timeline of the emergence of PSI, PSII and Cyanobacterial lineages. Age estimates
424 for PSI (Cardona, 2018), PSII (Cardona *et al.*, 2019), crown group Cyanobacteria
425 (Schirromeister *et al.*, 2015b), major clades and taxa (Sánchez-Baracaldo, 2015; Sánchez-
426 Baracaldo *et al.*, 2017). The timing of the Great Oxidation Event (GOE) (Bekker *et al.*, 2004),
427 Gunflint formation (Fralick *et al.*, 2011) and Neoproterozoic Oxidation Event (Och & Shields-
428 Zhou, 2012). Cartoons are not drawn according to scale. Ancestral forms of oxygenic
429 photosynthesis powered by homodimeric PSII and PSI emerged in the early Archean or early
430 Paleoproterozoic. D0 denotes an ancestral core subunit before the gene duplication that led to
431 D1 and D2; it is thought to have assembled into a primordial water-splitting photosystem. The
432 most recent common ancestor of Cyanobacteria inherited a heterodimeric photosystem shared
433 by all extant oxygenic phototrophs. Taxa with smaller cell diameter (basal lineages and
434 Microcyanobacteria) are shown at the bottom and larger cell diameter (Macrocyanobacteria)
435 at the top. Major Cyanobacterial clades radiated into many diverse forms after the GOE.
436 Marine planktonic Cyanobacteria evolved towards the end of the Precambrian, and the
437 Cretaceous.
438





Benthic & microbial mats

Planktonic

