

Table S1 Results of the *R. chingii* mitogenome

| Scaffold | Length(bp) | Depth(×) | Scaffold | Length(bp) | Depth(×) |
|----------|------------|----------|----------|------------|----------|
| 1 | 249,921 | 360.0 | 7 | 33,548 | 222.0 |
| 2 | 90,804 | 399.0 | 8 | 28,618 | 327.0 |
| 3 | 59,096 | 353.0 | 9 | 27,917 | 283.0 |
| 4 | 55,758 | 372.0 | 10 | 14,750 | 636.0 |
| 5 | 41,969 | 311.0 | 11 | 10,655 | 653.0 |
| 6 | 38,023 | 254.0 | 12 | 1,272 | 661.0 |

Table S2 Verification of 16 connection relationships in the *R. chingii* mitogenome

| Lable | Length | Average pident | Toal scaffold (>1000bp) | scaffolds support | E value < 1e-5 |
|-------|--------|----------------|----------------------------|-------------------|----------------|
| 4_8 | 56,758 | 99.70% | 501 | 10(score) | 100% |
| 4_9 | 56,758 | 99.70% | 501 | 10(score) | 100% |
| 7_1 | 34,548 | 99.78% | 502 | 1(sacffolds) | 100% |
| 7_3 | 34,548 | 99.77% | 310 | 20(score) | 100% |
| 10_4 | 15,750 | 99.71% | 500 | 65(scaffolds) | 100% |
| 10_5 | 15,750 | 99.72% | 500 | 77(sacffolds) | 100% |
| 10_7 | 15,750 | 99.72% | 500 | 88(scaffolds) | 100% |
| 10_9 | 15,750 | 99.72% | 500 | 71(scaffolds) | 100% |
| 11_1 | 11,655 | 99.77% | 500 | 217(scaffolds) | 100% |
| 11_2 | 11,655 | 99.76% | 500 | 254(scaffolds) | 100% |
| 11_6 | 11,655 | 99.78% | 500 | 231(scaffolds) | 100% |
| 11_8 | 11,655 | 99.77% | 500 | 213(sacffolds) | 100% |
| 12_2 | 2,272 | 99.82% | 500 | 500(scaffolds) | 100% |
| 12_3 | 2,272 | 99.78% | 500 | 500(scaffolds) | 100% |
| 12_5 | 2,272 | 99.87% | 500 | 500(scaffolds) | 100% |
| 12_6 | 2,272 | 99.80% | 500 | 500(scaffolds) | 100% |

Table S3 The codon uses and the RSCU value in the *R. chingii* mitogenome

| Amino acid | Codon | Frequency of use | RSCU | Amino acid | Codon | Frequency of use | RSCU |
|------------|-------|------------------|------|------------|-------|------------------|------|
| Phe | UUU | 492 | 1.14 | Tyr | UAU | 252 | 1.26 |
| | UUC | 368 | 0.86 | | UAC | 148 | 0.74 |
| | UUA | 278 | 1.18 | | UAA | 66 | 0.81 |
| | UUG | 286 | 1.21 | | UAG | 103 | 1.27 |
| Leu | CUU | 289 | 1.22 | His | CAU | 224 | 1.28 |
| | CUC | 181 | 0.77 | | CAC | 127 | 0.72 |
| | CUA | 244 | 1.03 | | CAA | 241 | 1.32 |
| | CUG | 140 | 0.59 | | CAG | 125 | 0.68 |
| Ile | AUU | 399 | 1.21 | Asn | AAU | 264 | 1.18 |
| | AUC | 314 | 0.96 | | AAC | 183 | 0.82 |
| | AUA | 273 | 0.83 | | AAA | 334 | 1.13 |
| | AUG | 318 | 1 | | AAG | 259 | 0.87 |
| Met | GUU | 235 | 1.28 | Asp | GAU | 232 | 1.26 |
| | GUC | 147 | 0.80 | | GAC | 136 | 0.74 |
| | GUA | 201 | 1.10 | | GAA | 352 | 1.30 |
| | GUG | 149 | 0.81 | | GAG | 188 | 0.70 |
| Val | UCU | 278 | 1.40 | Glu | UGU | 126 | 1.04 |
| | UCC | 206 | 1.04 | | UGC | 117 | 0.96 |
| | UCA | 224 | 1.13 | | UGA | 74 | 0.91 |
| | UCG | 170 | 0.85 | | Trp | UGG | 225 |
| Ser | CCU | 228 | 1.37 | Cys | CGU | 151 | 1.05 |
| | CCC | 136 | 0.82 | | CGC | 69 | 0.48 |
| | CCA | 188 | 1.13 | | CGA | 166 | 1.16 |
| | CCG | 115 | 0.69 | | CGG | 123 | 0.86 |
| Thr | ACU | 183 | 1.22 | Ser | AGU | 177 | 0.89 |
| | ACC | 144 | 0.96 | | AGC | 139 | 0.70 |
| | ACA | 163 | 1.09 | | AGA | 227 | 1.58 |
| | ACG | 108 | 0.72 | | AGG | 124 | 0.87 |
| Ala | GCU | 225 | 1.43 | Arg | GGU | 242 | 1.23 |
| | GCC | 142 | 0.90 | | GGC | 105 | 0.53 |
| | GCA | 152 | 0.96 | | GGG | 274 | 1.39 |
| | GCG | 112 | 0.71 | | GGG | 166 | 0.84 |

Table S4 Specific characteristics of MTPTs in the *R. chingii* mitogenome

| MTPT | Aligned length (bp) | Mitogenome | | Plastome | | Contained genes |
|------|---------------------|------------|---------|----------|---------|---|
| | | Start | End | Start | End | |
| 1 | 465 | 10,159 | 9,694 | 84,906 | 85,371 | partial-rpl2 ² |
| 2 | 162 | 36,394 | 36,232 | 30,344 | 30,510 | trnD-GUG ² |
| 3 | 180 | 36,876 | 37,056 | 45,239 | 45,419 | trnS-GGA ^{1,2} |
| 4 | 187 | 37,062 | 37,249 | 45,994 | 46,186 | partial-rps4 ² |
| 5 | 360 | 59,198 | 58,838 | 102,321 | 102,681 | partial-ycf68 ² , partial-trnL-CAA ² |
| 6 | 290 | 65,659 | 65,369 | 476 | 766 | - |
| 7 | 864 | 101,618 | 100,754 | 19,726 | 20,590 | partial-rpoC1 ² |
| 8 | 359 | 144,931 | 145,290 | 106,799 | 107,154 | - |
| 9 | 137 | 208,390 | 208,253 | 1,370 | 1,507 | - |
| 10 | 124 | 209,749 | 209,873 | 92,997 | 93,121 | - |
| 11 | 2829 | 214,094 | 211,265 | 102,977 | 105,806 | trnI-GAU ² , trnA-UGC ² |
| 12 | 232 | 219,103 | 219,335 | 21,268 | 21,500 | partial-rpoC2 ² |
| 13 | 262 | 292,436 | 292,174 | 101,616 | 101,879 | - |
| 14 | 4512 | 309,629 | 305,117 | 94,180 | 98,692 | trnL-CAA ^{1,2} , rps7 ^{1,2} , ndhB ^{1,2} |
| 15 | 132 | 345,919 | 345,787 | 4,269 | 4,401 | - |
| 16 | 288 | 399,455 | 399,743 | 101,060 | 101,348 | - |
| 17 | 1167 | 430,152 | 428,985 | 85,381 | 86,548 | partial-ccmC ¹ , rpl23 ^{1,2} , trnI-CAU ² |
| 18 | 2354 | 464,710 | 462,356 | 23,311 | 25,665 | partial-rpoB ² |
| 19 | 1206 | 465,904 | 464,698 | 21,619 | 22,825 | - |
| 20 | 653 | 632,530 | 631,877 | 66,587 | 67,251 | petG ² |
| 21 | 111 | 632,619 | 632,508 | 66,164 | 66,275 | - |
| 22 | 1401 | 634228 | 632,827 | 64,773 | 66,173 | psbJ ^{1,2} , psbL ^{1,2} , psbF ^{1,2} , psbE ^{1,2} |
| 23 | 242 | 700,268 | 700,026 | 1,162 | 1,405 | partial-psbA ² |
| 24 | 172 | 780,138 | 779,966 | 38,695 | 38,866 | partial-psaB ² |

Note: ¹, gene in mitogenome; ², gene in plastome; partial-, gene fragments exist in MTPTs.

Table S5 Shared genes and endemic genes in the three species (*R. chingii*, *P. chinensis*, *A. indica*)

| | mitogenome | | plastome | |
|---------------------|--|---|--|---|
| | share gene | Endemic gene | share gene | Endemic gene |
| <i>R. chingii</i> | | | | <i>accD, atpA, atpB, atpE, atpF, atpH, atpI, ccsA, cemA, matK, ndhA, ndhB, ndhC, ndhD, ndhE, ndhF, ndhG, ndhH, ndhI, ndhJ, ndhK, petA, petB, petD, petG, petL, petN, psaA, psaB, psaC, psaI, psaJ, psbA, psbB, psbC, psbD, psbE, psbF, psbH, psbI, psbJ, psbK, psbL, psbM, psbN, psbT, psbZ, rbcL, rpl32, rpoA, rpoB, rpoC1, rpoC2, rps15, ycf1, ycf3, ycf4, ycf15, ycf68</i> |
| | <i>atp1, atp4, atp6, atp8, atp9, ccmB, ccmC, ccmFc, ccmFn, cob, cox1, cox2, cox3, mttB, matR, nad1, nad2, nad3, nad4, nad4L, nad5, nad6, nad7, nad9, rpl12, rpl15, rpl10, rpl16, rps3, rps4, rps12, rps13, rps14</i> | <i>rps10, rps7, rpl23, sdh3, sdh4, ndhB, psbE, psbF, psbJ, psbL</i> | <i>clpP, rpl2, rpl14, rpl16, rpl20, rpl22, rpl23, rpl33, rpl36, rps2, rps3, rps4, rps7, rps8, rps11, rps12, rps14, rps16, rps18, rps19, ycf2</i> | |
| | | | | <i>atpA, atpB, atpE, atpF, atpH, atpI, cemA, infA, petA, petB, petD, petG, petL, petN, psaA, psaB, psaI, psaJ, psbA, psbB, psbC, psbD, psbE, psbF, psbH, psbI, psbJ, psbK, psbL, psbM, psbN, psbT, psbZ, rbcL, rpoA, rpoB, rpoC1, rpoC2, ycf3, ycf4</i> |
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| <i>P. chinensis</i> | | | | |
| <i>A. indica</i> | | - | | <i>accD, matK, rps15, ycf1</i> |

Table S6 Characterization of the sequence matrices used for organellar phylogenetic inference.

| | Total number of sites | Sites with alignment gaps or missing data | Invariable sites | Singleton variable sites | Parsimony informative sites |
|------------|-----------------------|---|------------------|--------------------------|-----------------------------|
| Mitogenome | 29,713 | 9.03% | 26,690 | 2,363 | 660 |
| Plastome | 82,350 | 26.72% | 67,326 | 10,599 | 4,465 |

Table S7 Characterizations of mitogenomes of 11 Lamiales species.

| Species | Family | Total length (bp) | Gene number | CDS number | GC% |
|---------------------------------|------------------|-------------------|-------------|------------|------|
| <i>Pedicularis chinensis</i> | Orobanchaceae | 225,612 | 62 | 37 | 44.4 |
| <i>Pedicularis kansuensis</i> | Orobanchaceae | 273,598 | 63 | 37 | 44.3 |
| <i>Castilleja paramensis</i> | Orobanchaceae | 495,499 | 68 | 36 | 43.5 |
| <i>Aeginetia indica</i> | Orobanchaceae | 420,362 | 55 | 33 | 43.5 |
| <i>Rehmannia chingii</i> | Orobanchaceae | 783,161 | 77 | 47 | 44.8 |
| <i>Rehmannia glutinosa</i> | Orobanchaceae | 547,032 | 71 | 44 | 45.0 |
| <i>Salvia miltiorrhiza</i> | Lamiaceae | 499,236 | 69 | 42 | 44.4 |
| <i>Utricularia reniformis</i> | Lentibulariaceae | 857,234 | 68 | 40 | 44.0 |
| <i>Aragoa cleefii</i> | Plantaginaceae | 365,824 | 55 | 34 | 44.9 |
| <i>Dorcoceras hygrometricum</i> | Gesneriaceae | 510,519 | 60 | 29 | 43.3 |
| <i>Osmanthus fragrans</i> | Oleaceae | 563,202 | 74 | 44 | 44.6 |

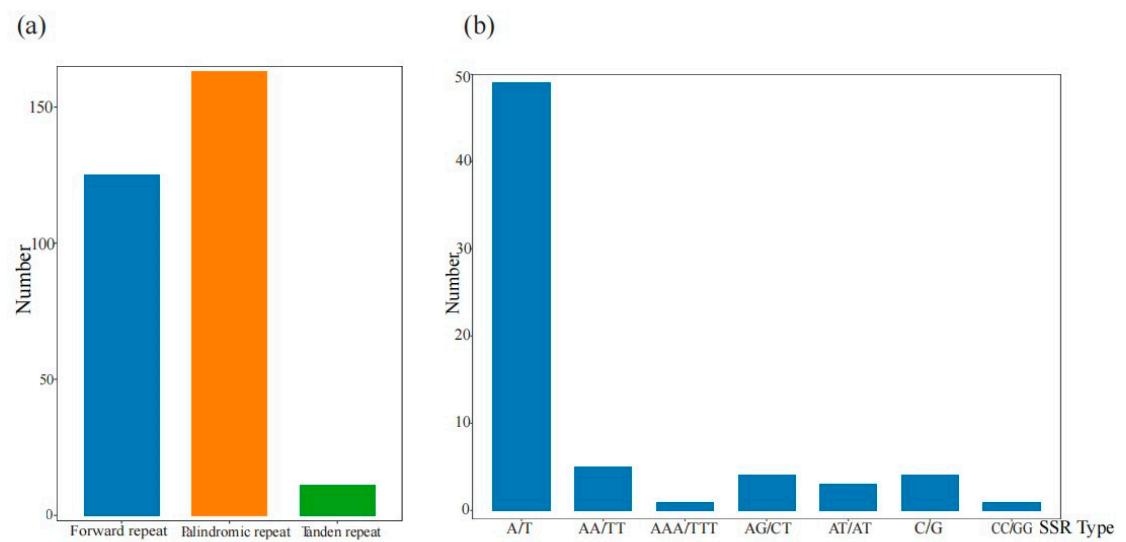


Figure S1. Repeat analysis of *R. chingii* mitogenome. (a) Repeat sequence statistics in the *R. chingii* mitogenome. (b) SSR statistics in the *R. chingii* mitogenome.