## **Supporting Information**

## Mau et al. 10.1073/pnas.1423447112

## **SI Materials and Methods**

Genetic Resources. Here, we analyzed 1,649 accessions (i.e., single samples from different populations per species) obtained from three pools of seed families: (i) 200 accessions of 11 Boechera taxa (Dataset S1), (ii) 75 accessions of 18 Boechera taxa (1), and (iii) 1,374 accessions of all available taxa, which covers 84 of the currently accepted 111 Boechera taxa. All seven major Boechera cpDNA-haplotype lineages (Boechera taxa of the three pools partially overlap) (Dataset S1) (2) were represented in the Boechera samples. In addition, nine taxa of neighboring genera of the tribe Boecheraea were included for all analyses (2, 3). We used a three-step approach to infer the reproductive mode of each genotype. First, accessions from seed pool *i* were grown in a common garden at the Leibniz Institute of Plant Genetics and Crop Plant Research (IPK) plant growth facility, and DNA was extracted using the Agencourt Chloropure DNA extraction kit (Beckman Coulter). Reproductive mode was determined by the flow cytometric seed screen (1, 4) of 10-24 seeds from each plant (Dataset S1). Diploids producing >50% seeds with diploid [2C = (1Cmaternal) + (1Cpaternal)] embryos and triploid [3C = (2Cmaternal) + (1Cpaternal)] endosperm were defined as sexual whereas those producing >50% seeds with any deviation from this particular embryo-endosperm ratio were defined as apomictic (1, 5, 6), providing us with "sexual" and "apomictic" reproductive-mode classes. Second, using Boechera accessions from seed pools *i* and *ii*, we conducted a PCR-based analysis for the presence/absence of the candidate marker gene for either male (UPGRADE2) (7) or female apomeiosis (APOLLO) (8). Third, we used dried herbarium material from which seeds could not be collected (pool iii) to perform a PCR-based screen for the presence/absence of either UPGRADE2 or APOLLO. Plant material representing 1,373 accessions for DNA analysis was obtained from herbarium accessions from Heidelberg University [Heidelberg Botanic Garden and Herbarium (HEID), Heidelberg; Marcus Koch, Department of Biodiversity and Plant Systematics; taxonomic information according to ref. 3; Dataset S1].

Processing and Analysis of DNA Sequences. PCR primers for a 645-bp fragment of the male-apomeiosis marker gene UPGRADE2 ("PC1pol1-L", 5'-CTTTTCCGTTGACTTTCCGACAAAT-3'; and "PC1pol1-R", 5'-TCGATCAATCTCATTCGGGATCTAT-3') (7) and of a 234-bp fragment spanning the apomixis-specific 5' UTR polymorphism of the female-apomeiosis marker gene APOLLO ("Lara5-F", 5'-CCTCATCGTACCGTTGCTTCTCTC-3'; and "TSP1-R", 5'-GATAGCCCCAAACTCCAAAATCGC-3') (8) were designed with Primer3 v0.4.0 (Fig. S1). PCR was performed in a volume of 10  $\mu$ L, using 10  $\mu$ M of each primer, 2.0 mM MgCl<sub>2</sub>, and 0.5 U of BioTaq polymerase (Bioline). The housekeeping gene ACTIN2 was used as external template control ("RTAct2T7-L", 5'-GTTCCACCACTGAGCACAATGTTACC-3'; and "RTAct2T7-R", 5'-AGTCTTGTTCCAGCCCTCTTTTG-TG-3'). The amplifications were run on a Mastercycler EP Gradient S (Eppendorf) under the following conditions: 5 min initial denaturation at 95 °C; 32 cycles of amplification with 30 s at 95 °C, 30 s at 60 °C, and 1 min at 72 °C; and 10 min of final elongation at 72 °C. PCR success was verified with agarose gel electrophoresis.

**Phylogenetic Distribution of UPGRADE2 and APOLLO.** (Supra) cpDNAhaplotype designations based on *trnL-F* sequence data (EU154066– EU154341; GenBank Nucleotide database, www.ncbi.nlm.nih. gov/nuccore) of 1,010 investigated accessions are available from ref. 2 (i.e., haplotypes collapsed into suprahaplotypes when sharing the same base order with exception for pseudogene-rich regions). Network reconstruction was conducted using the TCS 1.21 software with a connection limit of 95% (9) according to the parsimony analysis in ref. 2. Classification of accessions from lineages IV and V (Southeast United States) to either *Boechera* or to the closely related *Borodinia* is an ongoing debate (10, 11) and led to exclusion of 38 accessions from lineages IV and V from statistical analyses. Only taxa with a statistically valuable number of accessions ( $n \ge 10$ ) were used for statistical analyses using SPSS v20 (LEAD Technologies).

Niche Variation Models. The nearly total association between APOLLO presence and the apomixis phenotype (see *Results*) and the hypothesized association with unreduced egg formation (8) led us to use the presence of APOLLO as a surrogate for labeling a herbarium sample as apomictic. Sample coordinates of 97% (n = 1,595) of the 1,649 successfully screened Boechera accessions were taken from refs. 2 and 12. We used DIVA GIS v7.5 (www.diva-gis.org/) to calculate the geographic range area for species with at least five accessions in each of the two reproductive classes. For the geographic range of each reproductive class per species, we created a minimum convex polygon, clipped these polygons to North America (i.e., excluding accessions in Greenland), removed oceanic coverage, and calculated the area of each polygon in square kilometers (13). We used minimum convex polygons to estimate species-specific reproductive-mode geographic range because this approach provides a way to consistently calculate range across taxa. Calculations of species-specific niche models for apomicts and sexuals were performed with Maxent version 3.3.3 (default settings, replicates = 15, random seed, training set = 80%, test set = 20%, regularization multiplier = 1; convergence threshold = 0.00001, maximum iterations = 5,000) (14). For reasons of model stability only species with at least 10 observations in each reproductive-mode class were considered for Maxent niche models using the 2.5 arcminute (~5 km<sup>2</sup>) climate and elevation grids including all climatic layers (n = 19) from the WorldClim database (15). Maxent generated a threshold-independent, continuous output for climatic suitability range (0-1) of each sample subset based upon its biogeographic abundance. The model performance was then evaluated using the receiver operating characteristic (ROC) analysis (16) with the area under ROC curve (AUC) index (17). An AUC value of 0.5 indicates that the performance of the model meets randomness whereas values closer to 1.0 indicate better model performance. Map reconstructions were performed with DIVA GIS v7.5 (www.diva-gis.org/).

To statistically evaluate the true ecological distance between apomictic and sexual accessions under different constraining variables (ploidy and geographic distance) separately, species with at least five observations per reproductive-mode class and at least three observations for each ploidy class were used in a stepwise constrained correspondence analysis (CCA) (18) using the R programming environment version 3.1.1 (19) and the vegan package version 2.0-10 (20). To prevent over-fitting, bioclimatic variables with minor importance for each separate ecological-niche model were removed by a random-forest backward-elimination analysis of all 19 bioclimatic variables and elevation using the varSelRF package version 0.7-3 (21). Random forest generates multiple classification trees from bootstrap samples. Each time, a subset of the sample [i.e., out-of-bag (OOB) samples] is used to calculate an estimate of the classification error along the addition of trees to the forest. The selected variables are those that yield the smallest OOB error rates using standard parameters (ntree = 5,000, mtryFactor = 1) (21). The selected bioclimatic variables with clear biological significance (i.e., smallest OOB error rate) were added sequentially (first to last) to the CCA, which was performed with and without geographic distance as a partial constraint. Permutation tests for CCA (number of permutations = 10,000; implemented as *anova* function in ref. 20) under a reduced model were applied to calculate the significance of relationships between (*i*) eco-

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logical niche and reproductive mode including ploidy variation, (*ii*) ecological niche and ploidy including reproductive-mode variation, (*iii*) ecological niche and reproductive mode independently of ploidy, (*iv*) ecological niche and ploidy independently of reproductive mode, and (*v*) spatial distribution and reproduction independently of the ecological niche. The probability of targeted type 1 error ( $\alpha$ ) with a *P* value threshold of  $\alpha = 0.05$  was conservatively adjusted using Bonferroni correction (critical threshold for *P* values =  $\alpha^* \approx \alpha/M$ , M = number of independent tests) (22).

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**Fig. S1.** Structure of apomixis marker genes *APOLLO* (*A*) and *UPGRADE2* (*B*). Red pins on sequence structure denote priming sites of primers used for PCRbased screen of apomixis-specific sequence polymorphism (red arrows). Bac5 and Assembly 2 denote different genomic BAC DNA sites from the same apomictic individual; A001b and ES524\_2 denote the genomic DNA sequence of both factors, respectively, in apomictic accessions (i.e. apo allele); and S385h and ES612\_1 denote the genomic DNA sequence of both factors, respectively, in sexual accessions (i.e. sex allele) (1, 2).

- 1. Mau M, et al. (2013) The conserved chimeric transcript UPGRADE2 is associated with unreduced pollen formation and is exclusively found in apomictic Boechera species. *Plant Physiol* 163(4):1640–1659.
- 2. Corral JM, et al. (2013) A conserved apomixis-specific polymorphism is correlated with exclusive exonuclease expression in premeiotic ovules of apomictic boechera species. *Plant Physiol* 163(4):1660–1672.



Fig. S2. Geographic distribution of *Boechera* accessions with and without apomictic alleles of the marker genes. The PCR-based screen shows similar distributional ranges of *Boechera* accessions with *APOLLO* (*A*) and with *UPGRADE2* (*B*) compared with accessions lacking *APOLLO* (*C*) or *UPGRADE2* (*D*). (Scale bars: 1,000 km).

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Fig. S3. Maxent predictive ecological-niche models for single *Boechera* species. Partial geographic divergences between reproductive modes on species level were observed. Statistical analysis revealed that most of the ecological divergence between sexuals and apomicts on species level is not statistically significant. Only *Boechera retrofracta* and *Boechera williamsii* (Table 1) show true geographic parthenogenesis (i.e. without interfering ploidy variation). Habitat suitability is represented using different colors from low (green) to high (red). Strength of distribution differences is displayed for the surplus of apomicts (shades of green) and the surplus of sexuals (shades of red).



Fig. S4. Maxent predictive ecological-niche models for single *Boechera* species with ploidy as constraining variable. Statistically significant niche differentiation was observed between diploids and polyploids at genus-wide level and at species level. Habitat suitability is represented using different colors from low (green) to high (red). Strength of distribution differences is displayed for the surplus of apomicts (shades of green) and the surplus of sexuals (shades of red).

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	APO	077			UPGRA	DE2									Source	
Таха	Pres	Abs	2	%	Pres	Abs	2	%	175	۲	TrnL-F	2	MOR	Ref. 1	Ref. 2	FNA
Boechera arcuata	2	2	4	50.00	2	2	4	50.00			kd, ci	2				
Boechera atrorubens	0	-	-	0.00	0	-	-	0.00								
Boechera breweri	-	ი	10	10.00	0	10	10	0.00	gx, ha, kn	m	fy, fe, ci, if, at: fz, bu, ci	ω				
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Boechera californica	n ·	э į	γi	100.00	n i	эį	ηį	00.001	ev ,og	7 0	ci, bu	7 7				
Boechera canadensis	-	16	/1	5.88	0	/1	1	0.00	ko, kp, ma, mb, mc. md. sc. sd	×	tu, tv, tw, tx, ek, ei	و				
Boechera cobrensis	-	21	22	4.55	0	22	22	0.00	ad, gy, hk, hl,	7	ci, ig	2				
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Boechera collinsii Doochera collinsii	ת <del>,</del>	x		100.001	ת <del>י</del>	סת	<u>×</u> -	00.00	ae, co, n, I	4	רפ, נד, דץ	η	1			
Boechera consanguinea	- ‹			00.001	- a		- ,	00.001	_	•						
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Boechera dispar		۷ <u>:</u>	7 700	0.00	о с,	7 0	7 7	0.00	-	ç		ć				
Boechera divaricarpa	158	46	204	71.45	128	83	211	60.66	cj, ad, ay, az,	42	А, АF, АН, АЈ,	32				
									ba, bn, bs, bt,		AO, AS, AV, AW,					
									bw, bx, by, c,		AZ, B, BA, BC,					
									cw, dk, dr, ds,		CI, BD, BJ, BO,					
									e, eb, ec, ed,		BR, bs, BT, F,					
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									g, g.p.,, ., k, l, r, s,							
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Boechera divaricarpa	2	-	m	66.67	0	m	m	0.00	Ч	٢	X, Υ, CS	m				
imes Boechera retrofracta																
Boechera falcatoria	-	0	-	100.00	-	-	2	50.00	ee	-						
Boechera falcifructa	-	0	-	100.00	0	-	-	0.00	mq	٢						
Boechera fecunda	0	-	-	0.00	0	-	-	00.00			E	<del>, -</del>				
Boechera fendleri	σ	œ	17	52 94	13	4	17	76 47	ev for is kd	œ	ed er en f	~ ~				
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Boechera fernaldiana	m	7	10	30.00	-	6	10	10.00	il, op, pc, ok	4	hi, hk, ci, c	4				
ssp. fernaldiana									-		•					
Boechera fernaldiana	0	m	m	0.00	0	m	m	0.00	f, pn	2						
ssp. vivariensis									<del>.</del>							
Boechera formosa	-	8	6	11.11	-	∞	6	11.11	ad, lc, po, pp, pq	ъ	br, gs	2				

Table S1. PCR screen of apomixis marker allele presence and absence in 84 species of Boechera, three species each of Polytectenium and Sandbergia, two species of Cusickiella, and

Table S1. Cont.																
	APOI	077			UPGRA	DE2									Source	
Таха	Pres	Abs	2	%	Pres	Abs	2	%	175	Ζ	TrnL-F	z	MOR	Ref. 1	Ref. 2	FNA
Boechera glareosa	2	0	2	100.00	2	٦	m	66.67	δ	-	d	1				
Boechera glaucovalvula	0	S	S	00.0	0	9	9	0.00	nh, sp	2	hb, hc	2				
Boechera gracilipes	-	ъ	9	16.67	-	ъ	9	16.67	f	-						
Boechera gunnisoniana	-	-	2	50.00	-	-	2	50.00	pk, ad	2	ds	-				
Boechera hastatula	-	0	-	100.00	-	0	-	100.00								
Boechera holboellii	2	2	4	50.00	-	m	4	25.00								
Boechera howellii	-	2	m	33.33	0	9	9	0.00	pr	-	er	-				
Boechera inyoensis	9	-	7	85.71	9	-	7	85.71	ad, ar, i, mk, ml	ъ	ci, aa	2				
Boechera johnstonii	0	-	-	00.0	0	-	-	00.0	ev	-						
Boechera koehleri	0	∞	∞	00.0	0	∞	∞	0.00	ac ,kn ,mm ,sa	4	ee, gb, ci, gc	4				
Boechera laevigata	-	20	21	4.76	0	22	22	0.00	kf, kh, ki, kk,	12	ib, fl, ef, fg	4				
									no, np, nr, ns,							
									nt, nu, or, ot							
Boechera lasiocarpa	0	2	2	00.0	-	2	m	33.33	ad	-	ah	-				
Boechera lemmonii	∞	24	32	25.00	9	26	32	18.75	er, gx ,kl, km,	∞	dm, br, bu, ci,	∞				
									ly, lz, ps, pt		eh, fs, m, cw					
Boechera lignifera	24	S	29	82.76	20	6	29	68.97	ac, ad, ee, er,	13	u, by, b, ci, dt, ab, bu	7				
									gz, h, i, ib, ic,							
									id, ie, iw, ix							
Boechera lincolnensis	m	-	4	75.00	m	2	S	60.00	ev, pw, mu, mx, so	ß	ga, gr	2				
Boechera Iyallii	9	14	20	30.00	10	11	21	47.62	ab, ad, iy, iz, l, py, v	7	m, fh, ah,	7				
											as, dv, ft, bt					
Boechera macounii	8	m	11	72.73	8	m	1	72.73	iw, ad, h, il, lt	ъ						
Boechera microphylla	27	∞	35	77.14	30	7	37	81.08	ik, il, im, in, h,	∞	b, m, dy, c,	10				
									ka, kb, op		ci, fo, dw, dx,					
											dz, dy					
Boechera missouriensis	0	2	7	0.00	0	7	2	0.00	ll, lr, ls, nn, sg	ъ	fl, fg, hm	m				
Boechera nevadensis	0	-	-	00.0	0	-	-	0.00	хd	-						
Boechera ophira	0	-	-	0.00	0	٢	-	0.00								
Boechera oxylobula	0	∞	8	0.00	0	8	8	0.00	hc, pz, ra,g	4	c, ds, ci	m				
Boechera pallidifolia	19	16	35	54.29	33	2	35	94.29	ad, rb, gz, lf	4	ds, ci, fb,	9				
											bw, gd, do					
Boechera parishii	0	2	2	0.00	0	2	7	0.00	f	-	ci	-				
Boechera patens	0	2	2	0.00	0	m	m	0.00	st	-						
Boechera pauciflora	18	9	24	75.00	13	12	25	52.00	ar, h , hf	m	b, cc, ci, cl,	11				
											iw, ix, iy, kb,					
Boechera paupercula	0	Μ	m	0.00	0	m	m	0.00	rc ,v	2						
Boechera pendulina	4	26	30	13.33	LC.	27	32	15.63	ev f. a. kt. ni. rd	9	en ha el	11				
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	APOI	07.			UPGRA	DE2							Į	Š	ource	
Таха	Pres	Abs	N	%	Pres	Abs	N	%	175	N	TrnL-F	N	AOR Re	ef. 1	Ref. 2	FNA
Boechera pendulocarpa	Ø	32	40	20.00	10	32	42	23.81	ab, bt, bw, bx, eo, ep, eq ,ff, fg, g, h	5	U, BM, BN, BP, BU, BW, CK, CL, CO, CR, K, M, Q ,S ,U	15				
Boechera perennans	12	20	32	37.50	22	11	33	66.67	ad, ev, f, ku, ne, nf, pb, re, rf	ი	ab, ci, dr, ep, eq, f, ha	ø				
Boechera perstellata	0	m	m	0.00	0	m	m	0.00	se	-	fl					
Boechera pinetorum	61	21	82	74.39	44	38	82	53.66	ac, ad, aj, ar, au, cg, ch, ci, ck, dy, f, fk, ga, gh, h, i, z	17	AH, AS, AT, B, BM, BP, BY, C, CG, CI, CM, CQ, CX, F,J ,K, N, O, S, U	20				
Boechera pinzliae	0	2	2	0.00	0	2	2	00.00	гg	-						
Boechera platysperma	4	ы	ი	44.44	0	11	11	0.00	kv, my, mz, na, nb, rh	9	es, er, gv, gw, gx, gy	9				
Boechera polyantha	2	9	∞	25.00	2	10	12	16.67	h, ri	2	ci	-				
Boechera polyantha × Boechera retrofracta	7	0	2	100.00	7	0	7	100.00								
Boechera puberula	17	30	47	36.17	-	47	48	2.08	au, eu, it, iu, kx, ol, om, on, pa, rj, rk, sf, sw	13	cj, h, hs, ht, hu, m, o, s, u, y	10				
Boechera puberula × Boechera retrofracta	-	0	-	100.00	-	0	-	100.00								
Boechera pulchra	2	7	6	22.22	-	16	17	5.88	eu, h, ky, la, lb, lc, ld, nk, nl, rl, su	1	ci, s, hg, et, eu, ev, ew	2				
Boechera pusilla	2	0	2	100.00	2	0	2	100.00	f	-						
Boechera pygmaea	0	2	2	0.00	0	m	m	00.0			EX	-				
Boechera rectissima	2	9	∞	25.00	0	6	6	0.00	le, mp, z	m	ey, gl, gi, gk	4				
Boechera repanda	0	9 1	9 10	0.00	0	9	9	00.0	mr, rm, rn	m	ln, gm	7 5				
Boechera retrotracta	861	5	çć2	0 0 0	5	9	çç7	16.46	aa, ac, ad, au, bj, bt, ck, cl, cr, du, dx, dy, dz, er, eu, ev, ey, ez, f, fa, fb, fc, fd, fe, fk, gy, h, ha, i, r, y, z	ñ	AA, AC, AH, AG, B, BJ, BU, BX, BY, BZ, CB, CC, CD, CE, CG, Cl, CJ, CN, CQ, CS, CT, CU, CV, CW, CX, CY, E, hz, I, M, N, O, P, R, S, T, U, V, Y	ກ				
Boechera rigidissima	1	-	2	50.00	0	-	-	00.0	kv	-	pq	-				
Boechera schistacea	0	m	m	0.00	0	S	ß	00.0	ro, rp, sh	m	s, fa	2				
Boechera shockleyi	0	5	ß	00.0	0	5	ß	00.0	mn, mo	2	ge, ab	2				
Boechera shortii	0	5	2	0.00	0	9	9	0.00	lg	-	gh, z	2				

Table S1. Cont.																
	APOI	077			UPGRA	DE2									Source	
Таха	Pres	Abs	N	%	Pres	Abs	N	%	175	N	TrnL-F	N	MOR	Ref. 1	Ref. 2	FNA
Boechera sparsiflora	20	27	47	42.55	12	35	47	25.53	gx, h, ii ,lm , ou,c, f, i, lv, mf ,og ,rr, u	£	ci, b, iz, u, ka, p, ke, fd, fi cy, fk, bu, ga, as, fz, hh, fc	17				
Boechera sparsiflora × ? Boechera spatifolia	- 5	0 00	1	100.00 57.89	- 5	0 ∞	1 1	100.00 57.89								
Boechera species	19	Ø	27	70.37	15	12	27	55.56	az, bw, bx, h	4	AB, AH, AS, BJ, BU, BY, CC, ci, CI, dI, dn, hI. ie, L. M. U	16				
Boechera stricta	29	149	178	16.29	10	173	183	5.46	e, az, c, cm, cn, cq, d, dj, e, gz, I, m, r, rs, s, t, v	11	AD, ah, Al, Al, AK, AM, AN, AO, AP, AQ, AR, as, AU, av, AY, BA,	31				
											BB, BC, BD, BE, bf, bh, BJ, BK, BL, bs, CW, df, db, hv, ic					
Boechera stricta	-	0	-	100.00	-	-	2	50.00			с - -	-			I	
× Boechera retrofracta Boechera stricta	15	0	15	100.00	14	<del></del>	15	93.33								
× Boechera spatifolia Boechera subvious eidida	÷	٣	~	75.00	c	~	~		ac li hu lv	~	ي بو	ç				
Boechera suffrutescens	- m	n m	1 0	50.00	00	• ~	• ~	0.00	av, II, IW, IX ax, Ik, me	tΜ	db, fa, ff, fe	14				
Boechera tiehmii	-	0	٢	100.00	0	٢	-	0.00	er	٢	wh	-				
Boechera williamsii	m (	ω ·	9,	50.00 0.00	ω •	Μ	. e	50.00	ao, bt, iv	ω ·	hx, as	~ ~				
Boechera xylopoda Cusickiella doundasii	o c	- 4	- 7	00.0		04	— и	20.00	mw	-	gq	-				
Cusickiella quadricostata		· <del>-</del>	- 2	50.00	• 0	- 7	5 7	0.00								
Polyctenium fremontii	0	6	6	00.0	-	∞	6	11.11								
Polyctenium fremontii	0	-	-	0.00	0	-	-	0.00								
var. contertum Polvrtenium williamsiae	c	~	~	000	c	~	~	000								
Sandbergia perplexa	0	· <del>-</del>	· –	0.00	0		I	0.00								
S. perplexa var. lemhiensis	0	-	-	0.00	0	-	-	0.00								
Sandbergia whitedii	0	-	-	0.00	0	-	-	0.00								
Schoenocrambe linifolia	0	7	7	0.00	0	22	22	0.00								
Abe absent: ENA Flora of N	Amo	rica web	rita hann	in aflorac or	othrower a	lfC vuse o	ro id_1	Pictate tacto	0+ai JTI (C31001-bi ac	vert leave	MOB mode	of reproc	inction or	indicatod	Success in	

Abs, absent; FNA, Flora of North America website (www.efloras.org/browse.aspx?flora\_id=18start\_taxon\_id=104152); ITS, internal transcribed spacer; MOR, mode of reproduction as indicated by presence and absence of the apomictic APOLLO allele; pres, present. Red cells, apomictic taxa; yellow cells, sexual/apomictic taxa; blue cells, no designation.

1. Dobes CH, Mitchell-Olds T, Koch MA (2004) Extensive chloroplast haplotype variation indicates Pleistocene hybridization and radiation of North American Arabis drummondii, A. x divaricarpa, and A. holboellii (Brassicaceae). Mol Ecol 13(2):349-370. 2. Kiefer C, Koch MA (2012) A continental-wide perspective: The genepool of nuclear encoded ribosomal DNA and single-copy gene sequences in North American Boechera (Brassicaceae). PLoS ONE 7(5):e36491.

Table S2. Frequencies of sexual and apomictic Boechera across recent and ancient cpDNA haplotypes

			L	JPGRADE2					APOLLO		
cpDNA haplotype	Age, Mya	Noncarriers, N	Carriers, N	Noncarriers, %	Carriers, %	Ratio	Noncarriers, <i>N</i>	Carriers, N	Noncarriers, %	Carriers, %	Ratio
AB	0.7–2	2	2	0.010	0.012	0.8	3	1	0.018	0.005	3.5
В	0.7–1	8	12	0.039	0.072	0.5	6	14	0.035	0.071	0.5
BR	0.35–1	1	2	0.005	0.012	0.4	1	2	0.006	0.010	0.6
AH	0.35–1	48	46	0.236	0.277	0.9	38	54	0.224	0.274	0.8
BU	0.25-0.7	19	19	0.094	0.114	0.8	18	20	0.106	0.102	1.0
AS	0.25-0.7	87	49	0.429	0.295	1.5	70	66	0.412	0.335	1.2
CG	0.12-0.3	12	21	0.059	0.127	0.5	13	20	0.076	0.102	0.8
BY	Tip	26	15	0.128	0.090	1.4	21	20	0.124	0.102	1.2
Total no.	_	203	166	1.000	1.000	_	170	197	1.000	1.000	_
r <sup>2</sup>	—	_	—	_		0.281	—	—	_	—	0.499

The age estimations corresponding to the various cpDNA haplotypes were calculated in ref. 1. Mya, million years ago; Tip, cpDNA haplotypes at the tip of a strict consensus phylogenetic tree that is assembled from 10,000 maximum parsimonious trees.

1. Dobes CH, Mitchell-Olds T, Koch MA (2004) Extensive chloroplast haplotype variation indicates Pleistocene hybridization and radiation of North American Arabis drummondii, A. x divaricarpa, and A. holboellii (Brassicaceae). Mol Ecol 13(2):349–370.

Table S3. Species-specific habitat distribution variation

PNAS PNAS

				Geo	graphic iables		WWF k	piome	occup	ation,	% <sup>§</sup>		Se	election of	biovariables i	influential on habita	at distribution <sup>¶</sup>	
Species	MOR*	AUC <sup>†</sup> (training)	AUC <sup>†</sup> (test)	Range, log <sub>10</sub> km <sup>2</sup>	Latitude <sup>‡</sup>	4	5	9	∞	11	12	13	Elevation	Bio1	Bio3	Bio4	Bio12	Bio18
B. collinsii	Sex			6.11	49 (47, 50)	16.7	0.0	16.7	66.7	0.0	0.0	0.0	541 (345, 871)	3 (3, 4)	26 (25, 31)	1,103 (1,043, 1,200)	445 (401, 714)	208 (163, 235)
-	Apo	I		6.61	48 (48, 48)	66.7	11.1	11.1	11.1	0.0	0.0	0.0	66 (66, 309)	3 (3, 3) 2 (3, 3)	24 (24, 24)	1,051 (1,051, 1,051)	) 925 (448, 925)	254 (171, 254)
<i>b</i> . crandalli	Ano			5.44 2.85	39 (38, 39) 38 (38, 38)		55.5 53.3 5.5	0.0				00./ 2 66.7 2	(2391 (2,462, 2,660) 732 (2 386 2 732)	2 (2, 3) 2 (7 3)	41 (41, 41) 47 (42 42)	9/4 (935, 981) 889 (865–916)	500 (3/U, 500) 501 (397 519)	119 (112, 124) 141 (115 141)
B. divaricarpa	Sex	0.979	0.977	6.96	44 (41, 47)	18.0	66.7	5.1	5.1	2.6 (	0.0	5.1	,738 (216, 2,428)	- (-, -) 4 (2, 6)	37 (26, 43)	865 (726, 1,026)	526 (413, 783)	113 (73, 180)
	Apo	0.988	0.960	6.96	45 (42, 47)	11.9	66.4	7.0	4.9	0.7 (	0.0	9.8	,850 (334, 2,304)	3 (1, 5)	38 (27, 42)	842 (781, 1,023)	554 (456, 788)	136 (102, 216)
B. fendleri	Sex	I		5.63	36 (35, 37)	0.0	14.3	0.0	14.3	0.0	0.0	71.4 2	,010 (1,875, 2,718)	9 (7, 11)	43 (41, 44)	772 (734, 783)	375 (314, 436)	100 (90, 141)
	Apo	Ι		5.36	37 (36, 38)	0.0	25.0	0.0	0.0	0.0	0.0	75.0 2	,236 (1,691, 2,308)	8 (8, 9)	41 (38, 42)	818 (770, 840)	372 (307, 405)	94 (83, 114)
B. lemmonii	Sex	Ι		6.19 7 70	42 (38, 49)	0.0	100.0	0.0	0.0	0.0	0.0	0.0	,998 (2,230, 3,425)	-1 (-2, 1)	39 (34, 42)	788 (608, 810)	667 (606, 755)	143 (101, 185)
illert d	Apo	I		5.58 00	50 (47, 51) 40 (47 E1)	0.0	0.c/ of 7	0.0	0.0	0.0	0.0	20.02	,138 (1,559, 2,282) (138 (1,707 ), 2,282)	1 (0, 3)	32 (31, 38) 25 (27, 27)	802 (/06, 822) 701 /770 807)	685 (6/3, 929) 602 (666 767)	1/1 (101, 1/9)
b. Iyalili	Ano			5.00	49 (47, 49) 47 (47, 49)	0.0	100.00	0.0	0.0		0.0	0.0	,037 (1,702, 2,299) .132 (1.918, 2.295)	2 (-1, 3) 1 (-1, 2)	32 (32, 34)	741 (699, 814)	586 (519, 1.370)	173 (172, 126)
B. microphylla	Sex	I	Ι	4.84	42 (41, 42)	0.0	66.7	0.0	0.0	0.0	0.0	33.3 2	,551 (2,326, 2,664)	2 (2, 3)	37 (37, 37)	902 (860, 926)	364 (309, 511)	88 (74, 111)
	Apo	Ι	I	5.63	42 (41, 44)	0.0	22.2	0.0	0.0	0.0	0.0	77.8 1	,957 (1,772, 2,318)	5 (4, 6)	41 (40, 42)	787 (766, 843)	391 (353, 529)	77 (67, 102)
B. pallidifolia	Sex	0.999	1.000	4.96	39 (39, 41)	25.0	0.0	0.0	0.0	0.0	0.0	75.0 2	,069 (1,929, 2,233)	6 (5, 7)	41 (37, 41)	914 (906, 916)	313 (266, 378)	81 (74, 103)
	Apo	1.000	1.000	5.02	39 (39, 40)	16.7	0.0	0.0	0.0	0.0	0.0	83.3 1	,980 (1,778, 2,514)	6 (3, 7)	39 (37, 41)	896 (881, 992)	331 (271, 359)	102 (74, 131)
B. pauciflora	Sex	I	I	5.30	41 (41, 44)	0.0	66.7	0.0	0.0	0.0	0.0	33.3	,553 (1,423, 1,874)	6 (5, 7)	43 (40, 45)	725 (715, 769)	446 (405, 462)	66 (47, 87)
	Apo			5.44	41 (39, 42)	0.0	60.0	0.0	0.0	0.0	0.0	40.0	,911 (1,550, 2,169)	6 (5, 7)	44 (42, 45)	704 (690, 737)	444 (346, 547)	55 (48, 61)
B. pendulocarpa	Sex	Ι		6.07	45 (43, 51)	0.0	31.3	31.3	12.5	0.0	0.0	25.0 1	,912 (914, 2,507)	2 (0, 4)	37 (33, 38)	852 (813, 900)	441 (350, 535)	106 (97, 132)
	Apo			5.36	41 (39, 43)	0.0	37.5	0.0	0.0	0.0	0.0	62.5 2	,637 (2,176, 2,794)	2 (2, 5)	38 (37, 43)	825 (762, 919)	427 (334, 498)	87 (75, 115)
B. perennans	Sex .	1.000	0.962	5.77	37 (35, 38)	0.0	7.7	0.0	0.0	0.0	0.0	92.3 1	,708 (1,269, 1,970)	13 (9, 15)	42 (41, 44)	823 (772, 862)	312 (251, 403)	86 (62,105)
	Apo	0.991	0.989	5.34	37 (36, 38)	0.0	0.0	0.0	0.0	0.0	0.0	00.0	(271 (1,184, 1,833)	13 (9, 14) 5 (4 0)	(27, 40) (42) (42)	800 (782, 825) 701 (772, 825)	(113, 213) 238 (213, 277)	62 (50, 66)
p. pilletorati	Ano	0.992	0.989	0.47 6.67	(c+ ',c) ec 39 (38, 42)	0.0	50.0	2.1	4.2	0.0	0.0	50.0	,911 (1,233, 2,172) .015 (1.821, 2.420)	5 (4, 9) 6 (4, 8)	42 (41, 42)	791 (698, 840) 791 (698, 840)	384 (279, 548)	74 (50, 108) 74
B. puberula	Sex	0.999	0.998	5.45	41 (39, 42)	0.0	15.4	0.0	0.0	0.0	0.0	84.6 1	,927 (1,707, 2,142)	7 (6, 8)	43 (42, 45)	772 (734, 807)	292 (246, 337)	57 (47, 64)
	Apo	0.999	0.999	5.14	41 (40, 42)	0.0	0.0	0.0	0.0	0.0	0.0 1	00.0	,922 (1,716, 2,103)	7 (6, 7)	43 (42, 44)	747 (715, 782)	348 (295, 435)	55 (50, 61)
B. retrofracta	Sex	0.991	0.975	6.77	47 (43, 55)	6.2	56.9	16.9	1.5	6.2 (	0.0	18.5 1	,034 (622, 1,701)	4 (0, 7)	36 (28, 41)	880 (810, 1,002)	430 (347, 675)	108 (87, 154)
;	Apo	I		6.78	42 (39, 45)	1.0	55.1	4.1	5.1	2.0 (	0.0	37.8 2	,180 (1,604, 2,593)	3 (1, 5)	40 (38, 42)	850 (775, 887)	412 (346, 529)	102 (68, 132)
B. sparsiflora	Sex	0.996	0.995	6.13	41 (38, 42)	0.0	31.8	0.0	4.6	0.0	3.6	50.0 1	,568 (1,341, 2,038)	7 (6, 9)	43 (42, 45)	737 (708, 815)	356 (277, 406)	50 (39, 64)
	Apo	0.997	0.987	5.88	42 (40, 43)	0.0	33.3	0.0	0.0	0.0	5.6	61.1 1	,688 (1,193, 2,081) 	6 (5, 10) 2 (5, 1)	43 (38, 45)	749 (709, 842)	421 (328, 511)	64 (45, 76)
B. spatifolia	Sex	I		3.83 2.83	39 (39, 41) 20 (20 20)	I		I	I		I		,//4 (2,438, 2,804)	Z (2, 4)	41 (40, 42)	820 (814, 877)	398 (338, 422) 401 (330, 421)	(/cl. /cl) /tl) /tl) /tl) /tl) /tl) /tl) /tl) /t
	Apo	000	0	5.90	38 (38, 39) 12 (10 11)			4	0			v (	,//4 (2,/22, 2,//4)	Z (Z, 3)	41 (41, 41)	(1 68 ,028) 028	495 (379, 495)	188 (140, 188)
B. stricta	yex .	0.998	0.999	6.21 5.22	42 (40, 45)	/11/	64.0	9.0	9.0	0.9 0.9	0.0	19.8 2	,499 (2,025, 2,899)	2 (0, 3) 2 (0 3)	39 (37, 41)	829 (782, 870)	538 (434, 6/0)	13/ (109, 1/0)
	Apo	0.986	0/6.0	78.9 Co.c	(41, 46) 45 (41, 46)	44.4	42.9	16./	0.0	0.0	0.0	0.0	,848 (200, 2,/08) 200 (2 112 2 511)	3 (0, 7)	38 (28, 40)	906 (789, 995) 880 (841, 008)	650 (495, 8/3) 445 (770 464)	181 (138, 261) 112 (64 115)
b. Williamsii	xex	I	I	5.92 7.12	43 (43, 43)	0.0	100.0	0.0	0.0	0.0	0.0	0.0	,290 (2,143, 2,544) Foc (2 Foc 2 Coc)	(1, 0) 1	40 (38, 41)	889 (841, 908) 604 (660 000)	(194, 47) (379, 46)	(c11, (94, 115) 05, 104, 07)
All enorioe	Apo Sov	0 050	0 057	3.47 7.06	43 (43, 43) 11 (30 11)	0.0 9	100.0	0.0 10	0.0		0.0 C	0.0 k	(090'7 '09C'7) 00C' (01 1 2 2 760)	(7 /)   2 /2 /	3/ (3/, 38) 40 (37 43)	834 (880, 908) 827 (771 016)	203 (330, 390) 110 (336 613)	90 (84, 97) 103 (68 117)
All sheries	Yar ,	1000	100.0	00.7	(## '60' 1#		1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	0, 0	1 ( Ú (	j r	0.0		,3/4 (1,120, 2,403) 027 (1,100, 2,700)		(24,16) 04	(016 (17) 200		(141,00) 001
	Apo	C07.0	1.66.0	/.04	42 (39, 45)	0./	52.4	4.6	х. У	c. I	0.2	2 4.25	(026,2 ,402, 1) /20,	4 (2, 6)	41 (37, 42)	829 (128, 208)	438 (356, 603)	101 (67, 141)
*MOR, mode of r	eproduci	tion.																
<sup>†</sup> The model perfo	irmance v	was evalua	ited usi	ng the rec	eiver operatii	ng cha	racteris	tic (RC	)C) ani	alysis v	vith t	he area	under ROC curve (A	AUC) index.	. An AUC valu	ue of 0.5 indicates th	nat the performan	ce of the model
meets randomnes	s where	as values c	loser to	1.0 indici	ate better mo	del pe	rforma	nce. –	-, spec	ies wi	th n <	< 10 ob	servations in each re	eproductive	e-mode class	were not considered	d for Maxent niche	e models.

<sup>t</sup> bold letters denote significant differences between reproductive modes (Student's t test,  $\alpha = 0.05$ ).

<sup>6</sup>Biome 4, temperate broadleaf and mixed forests; biome 5, temperate conifer forests; biome 6, boreal forests/taiga; biome 8, temperate grasslands, savannas, and shrublands; biome 11, tundra; biome 12, Mediterranean forests, woodlands, and scrub; biome 13, deserts and xeric shrublands. Grey blocks denote major habitat for each species (>50%). Bold letters mark significant differences in WWF biome affiliation

Bio1, annual mean temperature; bio3, isothermality; bio4, temperature seasonality; bio12, annual precipitation; bio18, precipitation of warmest quarter; median (lower quartile, upper quartile). Bold letters between sexuals and apomicts (Fisher's exact test). —, no WWF biome information available.

denote significant differences between reproductive modes (Student's t test,  $\alpha = 0.05$ ).

Table S4. Comparison of genetic diversity (number of cpDNA haplotypes per number of individuals) among sexual and apomictic accessions per species illustrating variation between reproductive mode on species level and similar distribution ranges across species

	No. indivi	of duals	No. genot	of types	Ger dive	netic rsity
Таха	Аро	Sex	Аро	Sex	Аро	Sex
B. collinsii	8	5	1	3	0.13	0.60
B. divaricarpa	144	40	28	13	0.19	0.33
B. lemmonii	7	17	5	6	0.71	0.35
B. microphylla	20	5	9	4	0.45	0.80
B. pauciflora	12	6	7	6	0.58	1.00
B. pendulocarpa	7	26	4	12	0.57	0.46
B. perennans	8	10	4	4	0.50	0.40
B. pinetorum	52	15	18	10	0.35	0.67
B. puberula	14	23	6	7	0.43	0.30
B. retrofracta	109	67	27	20	0.25	0.30
B. sparsiflora	16	18	8	9	0.69	0.50
B. stricta	24	133	8	29	0.33	0.22
Mean	_	_		_	0.43	0.49
SE	_	_		_	0.05	0.07
Student's t test (P)	_	—		_	0.478	0.478

## **Other Supporting Information Files**

Dataset S1 (XLSX)