

Table S1. Correspondence of gene copy names in Fig.1 and gene ID in Phytozome

Name of <i>rbcS</i> gene copy in Fig.1	Gene ID in Phytozome database
Eucgr.K02223	<i>Eucalyptus_grandis_copy1</i>
Eucgr.B03013	<i>Eucalyptus_grandis_copy2</i>
Eucgr.J01502	<i>Eucalyptus_grandis_copy3</i>
GSVIVG01008288001	<i>Vitis_vinifera_copy1</i>
Kalax.0543s0033	<i>Kalanchoe_laxiflora_copy1</i>
Kaladp0039s0498	<i>Kalanchoe_fedtschenkoi_copy1</i>
Kalax.0216s0010	<i>Kalanchoe_laxiflora_copy2</i>
Kalax.0654s0003	<i>Kalanchoe_laxiflora_copy3</i>
Kaladp0442s0049	<i>Kalanchoe_fedtschenkoi_copy2</i>
Kalax.0039s0111	<i>Kalanchoe_laxiflora_copy4</i>
Migut.I00348	<i>Mimulus_guttatus_copy1</i>
Migut.D01471	<i>Mimulus_guttatus_copy2</i>
Migut.D01473	<i>Mimulus_guttatus_copy3</i>
gene17686v1.0hybrid	<i>Fragaria_vesca_copy1</i>
Prupe.3G157200	<i>Prunus_persica_copy1</i>
MDP0000252890	<i>Malus_domestica_copy1</i>
MDP0000524809	<i>Malus_domestica_copy2</i>
MDP0000731480	<i>Malus_domestica_copy3</i>
gene03736v1.0hybrid	<i>Fragaria_vesca_copy2</i>
Prupe.1G311400	<i>Prunus_persica_copy2</i>
MDP0000547788	<i>Malus_domestica_copy4</i>
MDP0000185022	<i>Malus_domestica_copy5</i>
MDP0000392485	<i>Malus_domestica_copy6</i>
Lus10017597.g	<i>Linum_usitatissimum_copy1</i>
Lus10033558.g	<i>Linum_usitatissimum_copy2</i>
Lus10009172.g	<i>Linum_usitatissimum_copy3</i>
Lus10028471.g	<i>Linum_usitatissimum_copy4</i>
Aqcoe3G038800	<i>Aquilegia_coerulea_copy1</i>
Aqcoe3G038900	<i>Aquilegia_coerulea_copy2</i>
Thhalv10019199m.g	<i>Eutrema_salsugineum_copy1</i>
Thhalv10019202m.g	<i>Eutrema_salsugineum_copy2</i>
Brara.B01696	<i>Brassica_rapa_copy1</i>
Brara.K01182	<i>Brassica_rapa_copy2</i>
Cagra.3694s0005	<i>Capsella_grandiflora_copy1</i>
Carubv10021016m.g	<i>Capsella_rubella_copy1</i>
Bostr.26959s0199	<i>Boechera_stricta_copy1</i>
AT1G67090	<i>Arabidopsis_thaliana_copy1</i>
AL2G25460	<i>Arabidopsis_lyrata_copy1</i>
Araha.1584s0003	<i>Arabidopsis_halleri_copy1</i>
Thhalv10027955m.g	<i>Eutrema_salsugineum_copy3</i>
Brara.D00896	<i>Brassica_rapa_copy3</i>
Bol040168	<i>Brassica_oleracea_capitata_copy1</i>
Bol040169	<i>Brassica_oleracea_capitata_copy2</i>
Brara.D00895	<i>Brassica_rapa_copy4</i>
Bol040165	<i>Brassica_oleracea_capitata_copy3</i>
Brassica_rapa.D01185	<i>Brassica_rapa_copy5</i>
Brassica_rapa.G01432	<i>Brassica_rapa_copy6</i>
Carubv10005847m.g	<i>Capsella_rubella_copy2</i>
Carubv10007296m.g	<i>Capsella_rubella_copy3</i>
Carubv10007166m.g	<i>Capsella_rubella_copy4</i>
Bostr.12645s0002	<i>Boechera_stricta_copy2</i>
Bostr.12645s0001	<i>Boechera_stricta_copy3</i>

Bostr.12645s0004	<i>Boechera_stricta_copy4</i>
AT5G38430	<i>Arabidopsis_thaliana_copy2</i>
AT5G38420	<i>Arabidopsis_thaliana_copy3</i>
AT5G38410	<i>Arabidopsis_thaliana_copy4</i>
AL7G52150	<i>Arabidopsis_lyrata_copy2</i>
AL7G52160	<i>Arabidopsis_lyrata_copy3</i>
Araha.19953s0004	<i>Arabidopsis_halleri_copy2</i>
AL7G52170	<i>Arabidopsis_lyrata_copy4</i>
Araha.19953s0005	<i>Arabidopsis_halleri_copy3</i>
evm.TU.supercontig_282.14	<i>Carica_papaya_copy1</i>
Ciclev10012893m.g	<i>Citrus_clementina_copy1</i>
27524.t000006	<i>Ricinus_communis_copy1</i>
evm.TU.supercontig_1.37	<i>Carica_papaya_copy2</i>
evm.TU.supercontig_1.38	<i>Carica_papaya_copy3</i>
Thecc1EG012342	<i>Theobroma_cacao_copy1</i>
29974.t000003	<i>Ricinus_communis_copy2</i>
Manes.05G137400	<i>Manihot_esculenta_copy1</i>
Manes.01G011500	<i>Manihot_esculenta_copy2</i>
Thecc1EG009873	<i>Theobroma_cacao_copy2</i>
Thecc1EG009872	<i>Theobroma_cacao_copy3</i>
Thecc1EG019454	<i>Theobroma_cacao_copy4</i>
Gorai.001G201800	<i>Gossypium_raimondii_copy1</i>
Gorai.007G181300	<i>Gossypium_raimondii_copy2</i>
Gorai.007G181400	<i>Gossypium_raimondii_copy3</i>
Potri.017G114600	<i>Populus_trichocarpa_copy1</i>
SapurV1A.0101s0240	<i>Salix_purpurea_copy1</i>
Potri.004G100000	<i>Populus_trichocarpa_copy2</i>
SapurV1A.0315s0080	<i>Salix_purpurea_copy2</i>
30167.t000038	<i>Ricinus_communis_copy3</i>
Ciclev10023403m.g	<i>Citrus_clementina_copy2</i>
Solyc02g085950.2	<i>Solanum_lycopersicum_copy1</i>
PGSC0003DMG400012666	<i>Solanum_tuberosum_copy1</i>
PGSC0003DMG400026409	<i>Solanum_tuberosum_copy2</i>
Solyc03g034220.2	<i>Solanum_lycopersicum_copy2</i>
PGSC0003DMG400019584	<i>Solanum_tuberosum_copy3</i>
Solyc02g063150.2	<i>Solanum_lycopersicum_copy3</i>
PGSC0003DMG400024182	<i>Solanum_tuberosum_copy4</i>
Medtr7g007230	<i>Medicago_truncatula_copy1</i>
Medtr7g007200	<i>Medicago_truncatula_copy2</i>
Medtr7g007120	<i>Medicago_truncatula_copy3</i>
Medtr7g007220	<i>Medicago_truncatula_copy4</i>
Medtr7g007210	<i>Medicago_truncatula_copy5</i>
Tp57577_TGAC_v2_gene32455	<i>Trifolium_pratense_copy1</i>
Tp57577_TGAC_v2_gene32462	<i>Trifolium_pratense_copy2</i>
Medtr6g018300	<i>Medicago_truncatula_copy6</i>
Medtr6g018310	<i>Medicago_truncatula_copy7</i>
Phvul.004G064800	<i>Phaseolus_vulgaris_copy1</i>
Phvul.004G073400	<i>Phaseolus_vulgaris_copy2</i>
Phvul.004G073450	<i>Phaseolus_vulgaris_copy3</i>
Glyma.13G046200	<i>Glycine_max_copy1</i>
Glyma.19G046900	<i>Glycine_max_copy2</i>
Glyma.19G046800	<i>Glycine_max_copy3</i>
Glyma.19G046600	<i>Glycine_max_copy4</i>
Glyma.18G296900	<i>Glycine_max_copy5</i>
Glyma.14G089500	<i>Glycine_max_copy6</i>

Glyma.08G365300	<i>Glycine_max_copy7</i>
Glyma.18G182200	<i>Glycine_max_copy8</i>
Glyma.18G182300	<i>Glycine_max_copy9</i>
Sobic.005G042000	<i>Sorghum_bicolor_copy1</i>
GRMZM2G098520	<i>Zea_mays_copy1</i> (Ensembl-18)
Zm00008a017851	<i>Zea_mays_copy1</i> (PH207 v1.1)
GRMZM2G113033	<i>Zea_mays_copy2</i> (Ensembl-18)
Zm00008a008283	<i>Zea_mays_copy2</i> (PH207 v1.1)
Pavir.Cb01387	<i>Panicum_virgatum_copy1</i>
Pavir.J32704	<i>Panicum_virgatum_copy2</i>
Pavir.Ca02105	<i>Panicum_virgatum_copy3</i>
Pavir.Cb01593	<i>Panicum_virgatum_copy4</i>
Pahal.C03268	<i>Panicum_hallii_copy1</i>
Pahal.C03271	<i>Panicum_hallii_copy2</i>
Pahal.C03575	<i>Panicum_hallii_copy3</i>
Pahal.C03582	<i>Panicum_hallii_copy4</i>
Pahal.C03269	<i>Panicum_hallii_copy5</i>
Seita.3G312200	<i>Setaria_italica_copy1</i>
Sevir.3G315200	<i>Setaria_viridis_copy1</i>
Seita.3G312000	<i>Setaria_italica_copy2</i>
Seita.3G312400	<i>Setaria_italica_copy3</i>
Sevir.3G319300	<i>Setaria_viridis_copy2</i>
Sevir.3G315400	<i>Setaria_viridis_copy3</i>
Seita.3G269500	<i>Setaria_italica_copy4</i>
Sevir.3G276100	<i>Setaria_viridis_copy4</i>
Seita.3G269600	<i>Setaria_italica_copy5</i>
Sevir.3G276200	<i>Setaria_viridis_copy5</i>
LOC_Os12g17600	<i>Oryza_sativa_copy1</i>
LOC_Os12g19470	<i>Oryza_sativa_copy2</i>
LOC_Os12g19381	<i>Oryza_sativa_copy3</i>
Bradi5g04080	<i>Brachypodium_distachyon_copy1</i>
Brast09G038200	<i>Brachypodium_stacei_copy1</i>
Bradi3g26385	<i>Brachypodium_distachyon_copy2</i>
Brast03G114700	<i>Brachypodium_stacei_copy2</i>
Bradi3g26391	<i>Brachypodium_distachyon_copy3</i>
Bradii4g08500	<i>Brachypodium_distachyon_copy4</i>
Brast10G096300	<i>Brachypodium_stacei_copy3</i>
Bradi4g08800	<i>Brachypodium_distachyon_copy5</i>
Brast10G107800	<i>Brachypodium_stacei_copy4</i>

Table S2. Minimum number of *rbcS* gene copies per species in angiosperms

	lineage1	lineage2
<i>Aquilegia coerulea</i>	2	1
<i>Arabidopsis halleri</i>	3	0
<i>Arabidopsis lyrata</i>	4	0
<i>Arabidopsis thaliana</i>	4	0
<i>Brassica oleracea capitata</i>	3	0
<i>Boechera stricta</i>	4	0
<i>Brassica rapa</i>	6	0
<i>Brachypodium distachyon</i>	5	0
<i>Brachypodium stacei</i>	4	0
<i>Capsella grandiflora</i>	1	0
<i>Carica papaya</i>	3	1
<i>Capsella rubella</i>	4	0
<i>Citrus clementina</i>	2	1
<i>Citrus sinensis</i>	0	1
<i>Eucalyptus grandis</i>	3	1
<i>Eutrema salsugineum</i>	3	0
<i>Fragaria vesca</i>	2	1
<i>Glycine_max</i>	9	1
<i>Gossypium raimondii</i>	3	1
<i>Kalanchoe fedtschenkoi</i>	2	0
<i>Kalanchoe laxiflora</i>	4	0
<i>Linum usitatissimum</i>	4	2
<i>Malus domestica</i>	6	0
<i>Manihot esculenta</i>	2	1
<i>Mimulus guttatus</i>	3	1
<i>Medicago truncatula</i>	7	1
<i>Oryza sativa</i>	3	1
<i>Panicum hallii</i>	5	1
<i>Prunus persica</i>	2	1
<i>Populus trichocarpa</i>	2	1
<i>Panicum virgatum</i>	4	0
<i>Phaseolus vulgaris</i>	3	0
<i>Ricinus communis</i>	3	1
<i>Sorghum bicolor</i>	1	0
<i>Setaria italica</i>	5	1
<i>Solanum lycopersicum</i>	3	1
<i>Salix purpurea</i>	2	1
<i>Solanum tuberosum</i>	4	1
<i>Setaria viridis</i>	5	0
<i>Theobroma cacao</i>	4	1
<i>Trifolium pratense</i>	2	1
<i>Vitis vinifera</i>	1	1
<i>Zea mays</i>	4	0
Total number of gene copies	146	25
Total number of species	42	24

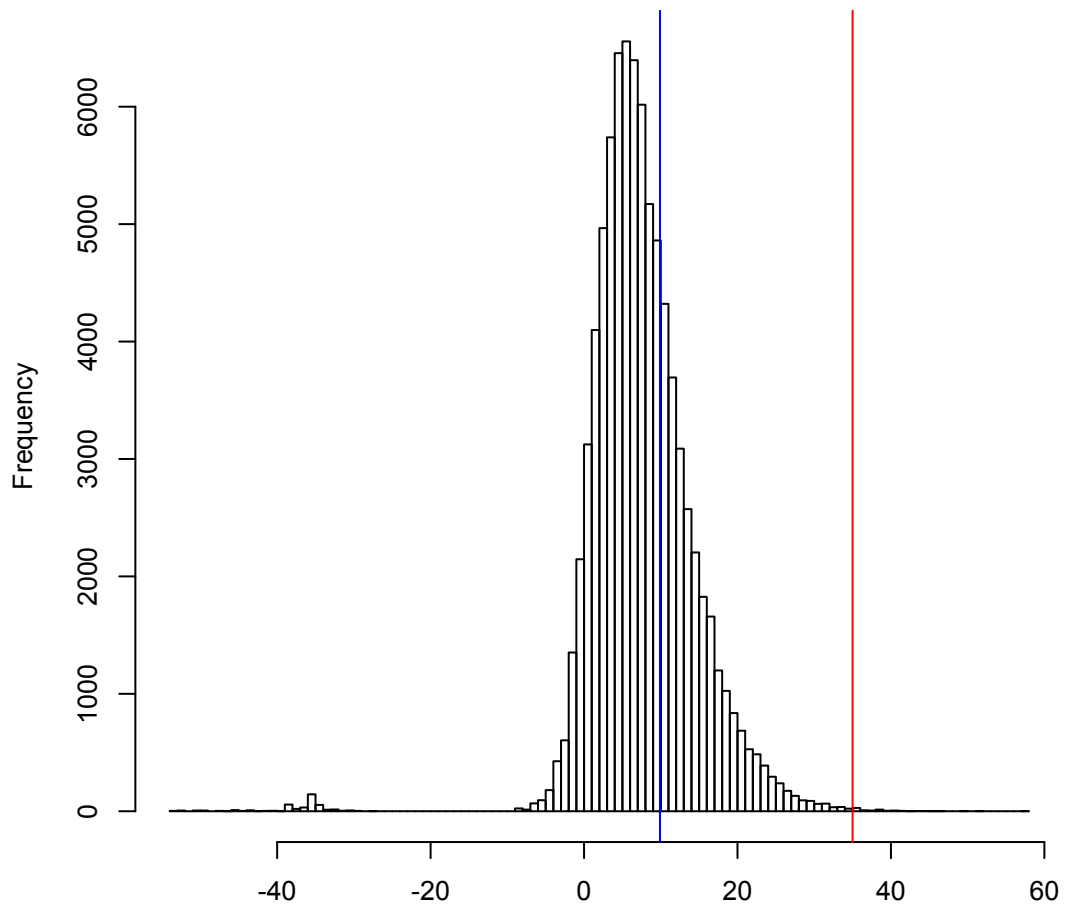
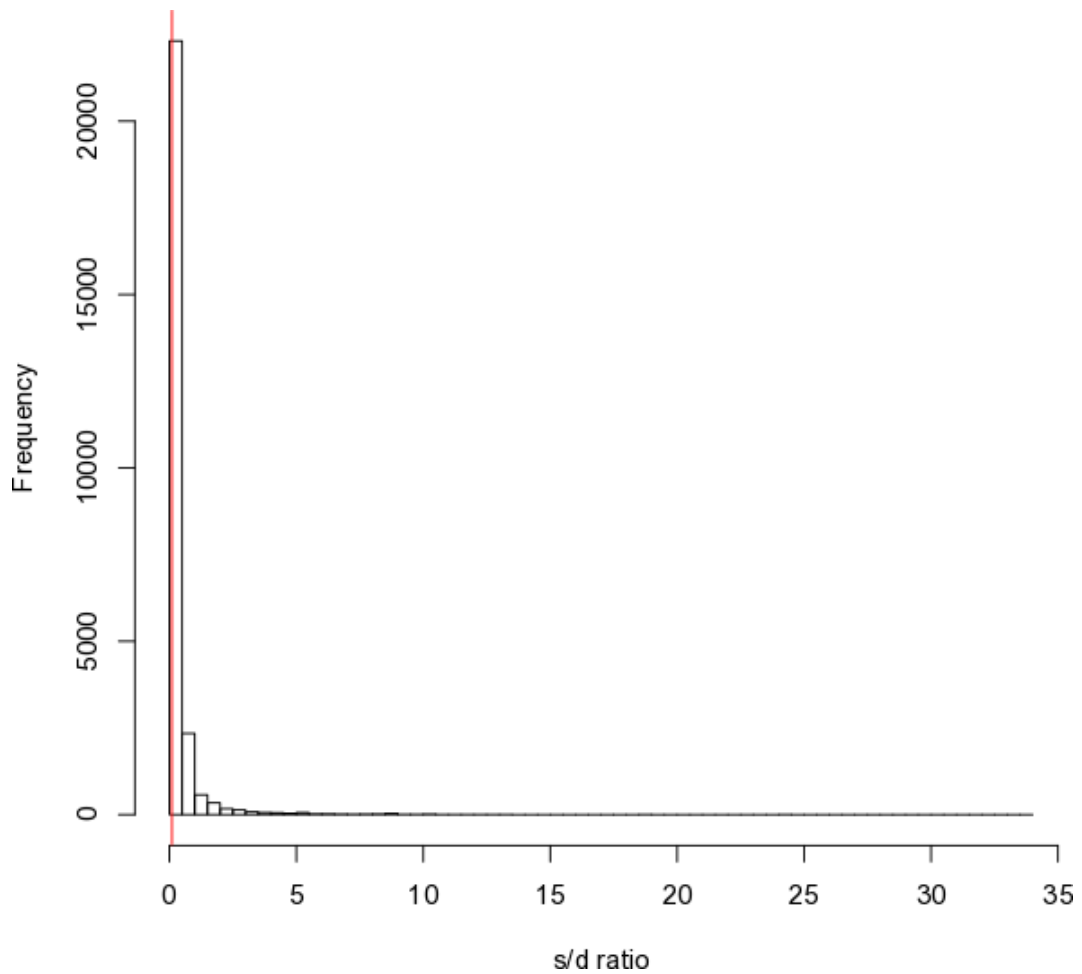
A.**B.**

Fig. S1. A) dAIC distribution of frequency of coevolving profiles by Coev model (Blue line: dAIC=9.893, Red line: dAIC=35). B) s/d ratio distribution of frequency of coevolving profiles by Coev model filtered by dAIC more than 9.893 (Red line: s/d ratio=0.1).

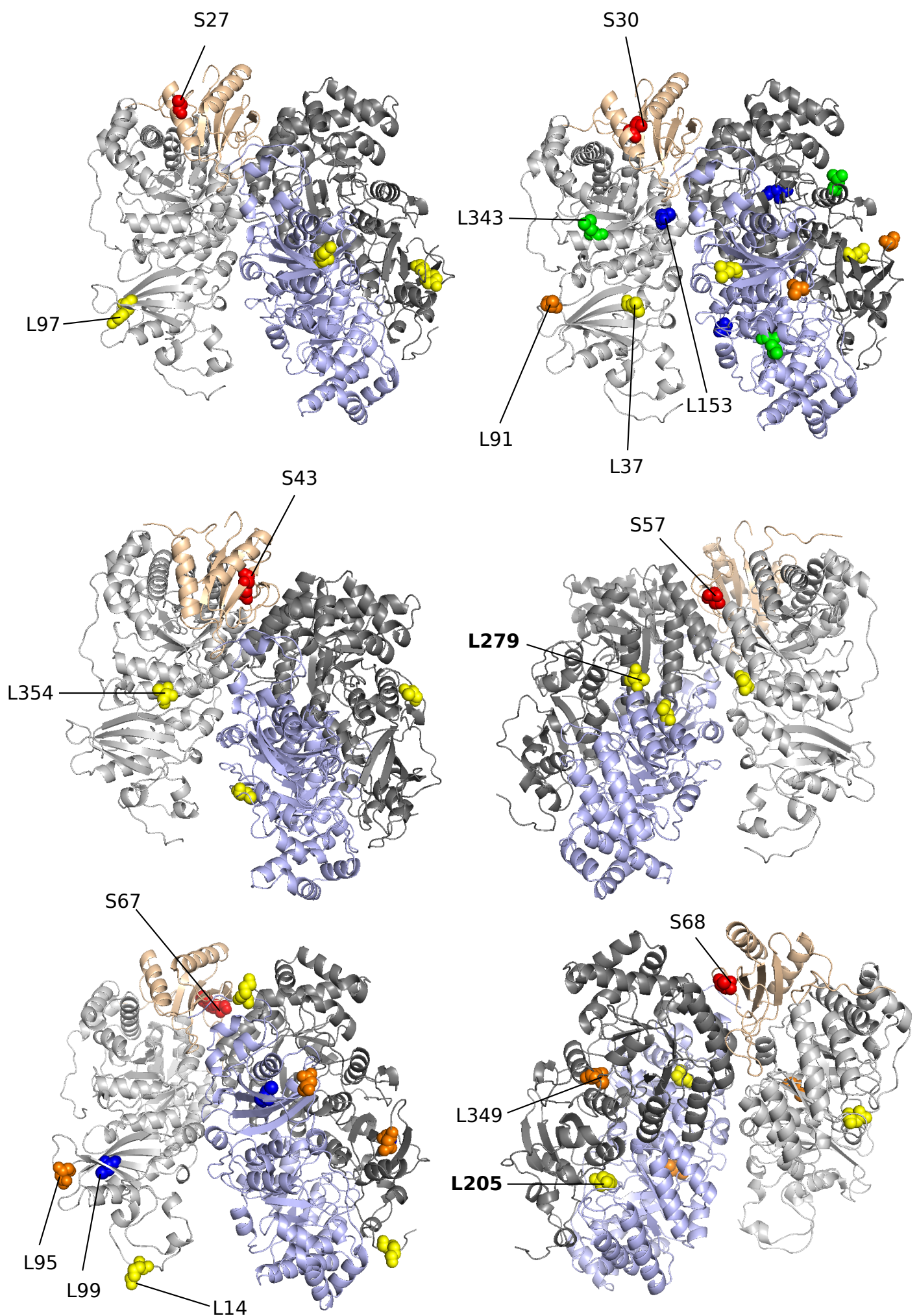


Fig. S2. A. The residues of RBCS and RBCL under coevolution plotted to known RuBisCO structure of spinach (1RCX of Protein Data Bank; Taylor et al., 1997).

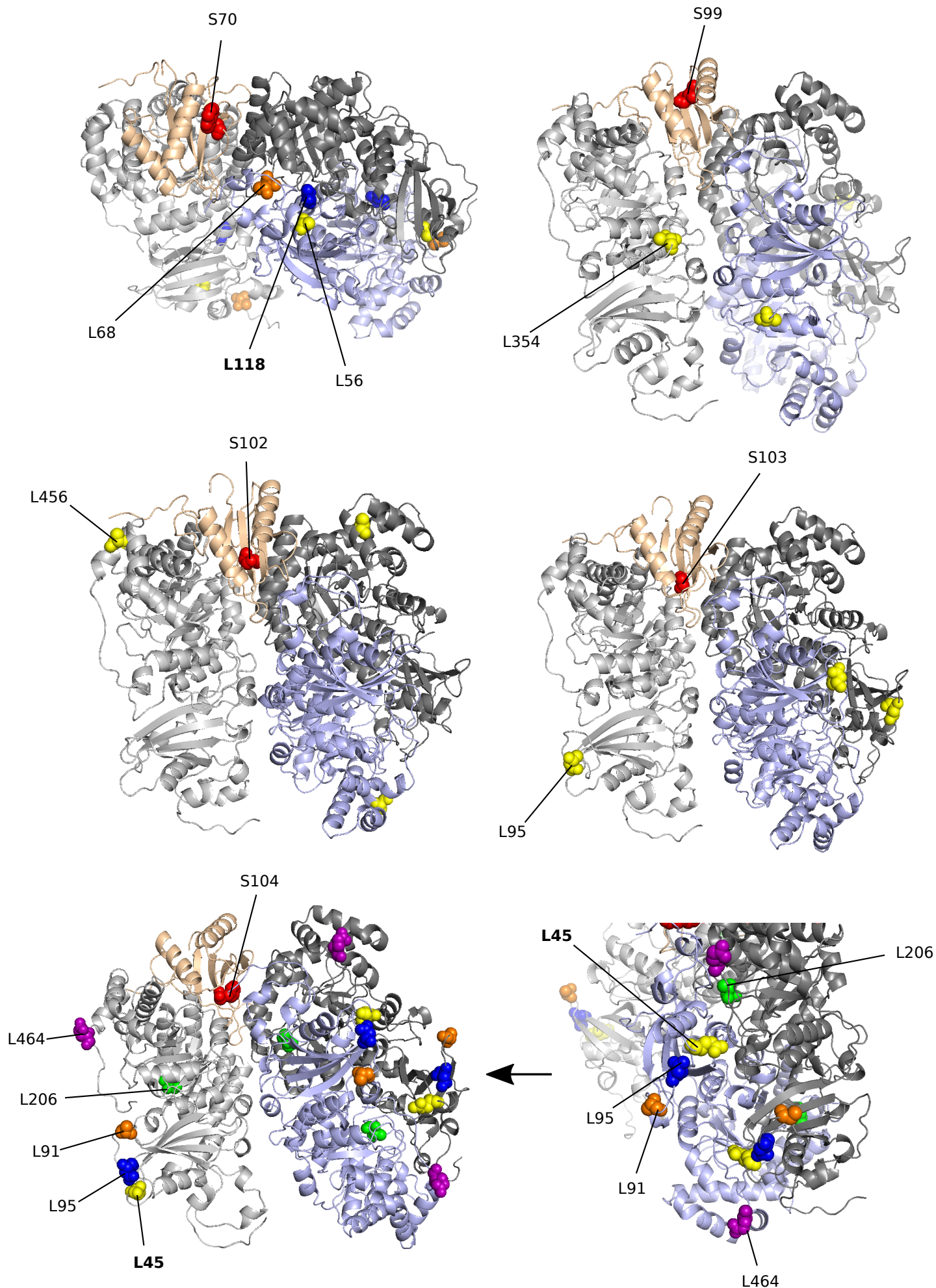


Fig. S2. B. The residues of RBCS and RBCL under coevolution plotted to known RuBisCO structure of spinach (1RCX of Protein Data Bank; Taylor et al., 1997).

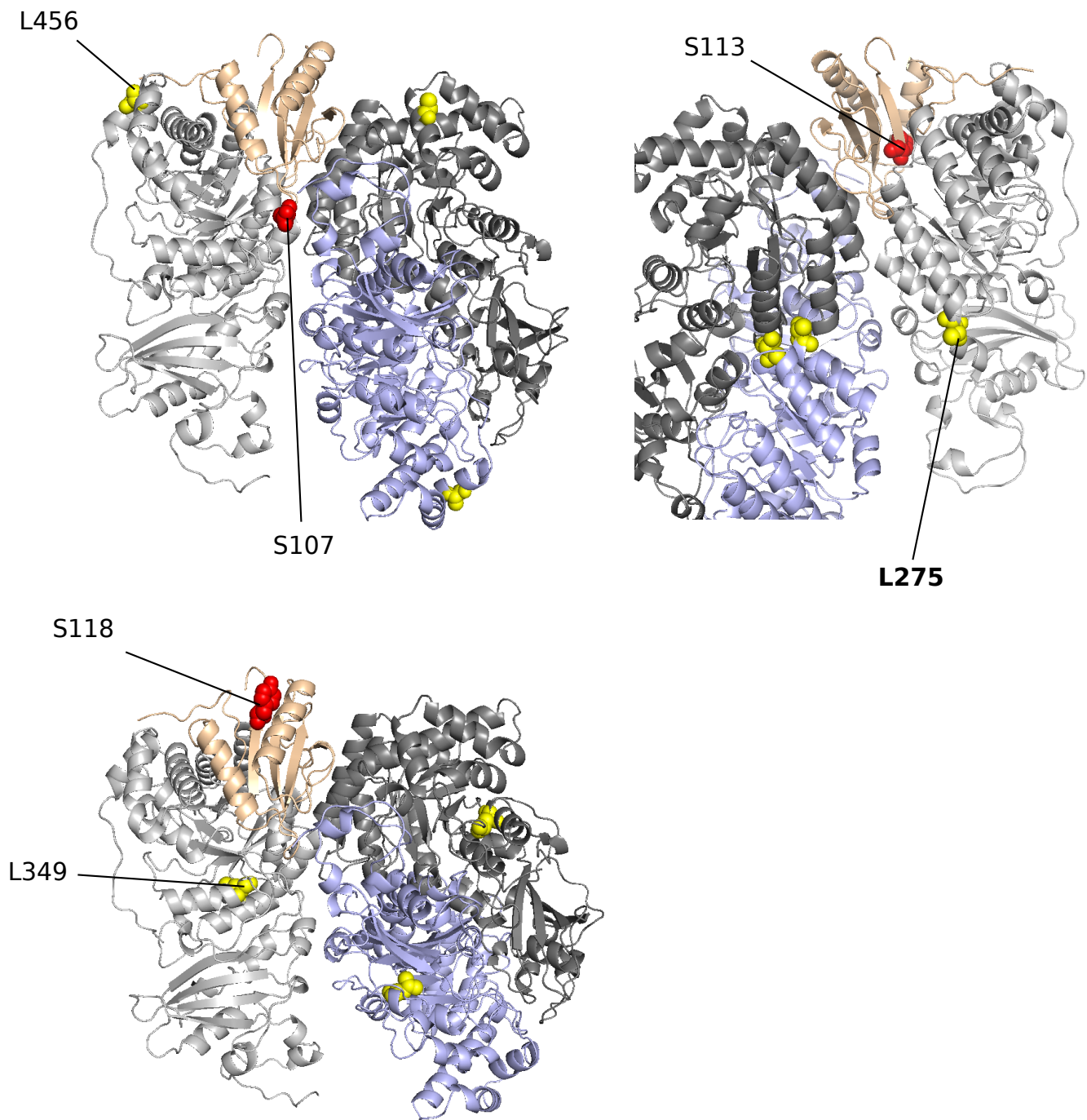


Fig. S2. C. The residues of RBCS and RBCL under coevolution plotted to known RuBisCO structure of spinach (1RCX of Protein Data Bank; Taylor et al., 1997).