

Supplementary data for article:

Smiljanic, K.; Apostolovic, D.; Trifunovic, S.; Ognjenovic, J.; Perusko, M.; Mihajlovic, L.; Burazer, L.; van Hage, M.; Cirkovic Velickovic, T. Subpollen Particles Are Rich Carriers of Major Short Ragweed Allergens and NADH Dehydrogenases: Quantitative Proteomic and Allergomic Study. *Clinical and Experimental Allergy* **2017**, *47* (6), 815–828.

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Table S5. Label free quantification results of total (TOT), aqueous (APE) and sub-pollen particle (SPI

Green color cell denotes officially recognized allergen, identified via shotgun proteomics (in so allergen isoform XIC curve area contributed to the sum of the XIC curve areas creating aller allergome within proteome for each pollen fraction shown at the end of th				
Accession	Description	Protein Group	Protein ID	TOT Area under XIC curve
Q0PUV7	(E)-4-hydroxy-3-methylbut-2-enyl diphosphate synthase	138	1482	0.0E+00
I6RE61	(E)-beta-ocimene synthase chloroplastic OS=Matricaria c	123	1209	1.2E+05
G8CUD5	Actin (Fragment) OS=Lactuca sativa PE=3 SV=1	31	17	3.9E+05
G5EN35	Actin OS=Chrysanthemum seticuspe f. boreale GN=CsAct	20	16	4.7E+05
E0D6S0	Actin OS=Gynura bicolor GN=GbACT PE=2 SV=1	25	18	1.5E+05
A5HML4	Adenosylhomocysteinase OS=Chrysanthemum morifoliu	104	7518	0.0E+00
V9VA11	Alcohol dehydrogenase 1A (Fragment) OS=Podospermun	96	203	1.4E+05
A0A0K1Z644	Alcohol dehydrogenase 1A (Fragment) OS=Tragopogon p	43	121	7.8E+04
D4NYE5	Ascorbate peroxidase 2-like protein (Fragment) OS=Trag	73	175	3.3E+05
W0FGD1	ATP synthase subunit alpha OS=Helianthus annuus GN=a	87	115	1.4E+05
C0SU64	Auxin efflux carrier component OS=Zinnia violacea GN=Zi	135	6562	0.0E+00
Q40751	Calreticulin (Fragment) OS=Parthenium argentatum GN=	40	8257	8.9E+05
Q8SA59	Carbohydrate oxidase OS=Helianthus annuus PE=4 SV=1	144	2044	0.0E+00
Q2KN26	Calcium-binding protein isoallergen 2 OS=Ambrosia arter	241	15777	0.0E+00
Q69AB6	CC-NBS-LRR-like protein (Fragment) OS=Helianthus annu	120	1149	1.6E+04
V5LU01	Cysteine protease OS=Ambrosia artemisiifolia PE=2 SV=1	22	34	5.3E+06
Q38678	Cysteine proteinase inhibitor OS=Ambrosia artemisiifolia	89	215	8.7E+04
P00069	Cytochrome c OS=Guizotia abyssinica PE=1 SV=1	65	412	0.0E+00
Q6S4N3	Cytochrome c OS=Helianthus annuus PE=2 SV=1	56	266	1.3E+05
A0A0M4JA76	Elongation factor 1-alpha OS=Cichorium intybus GN=EF1;	64	49	9.2E+05
Q9SC12	Eukaryotic translation initiation factor 5A OS=Senecio vei	126	408	7.2E+04
A1BLL7	Glucose-6-phosphate isomerase OS=Helianthus annuus C	49	213	5.1E+04
A0A0P0A367	Glyceraldehyde 3-phosphate dehydrogenase (Fragment)	38	40	1.2E+06
R4JCP3	Glyceraldehyde-3-phosphate dehydrogenase (Fragment)	69	56	9.8E+04
E0D6S1	Glyceraldehyde-3-phosphate dehydrogenase OS=Gynura	39	28	3.5E+05
G8XWY8	Glyceraldehyde-3-phosphate dehydrogenase OS=Mikania	42	39	4.4E+04
T1WLF9	Gly-rich RNA binding protein (Fragment) OS=Helianthus a	142	942	1.0E+04
A0A059XD04	Heat shock protein 70 OS=Chrysanthemum indicum PE=2	59	86	2.3E+05
O04223	HSP70-related protein (Fragment) OS=Helianthus annuus	112	395	1.2E+05
Q84ZX5	Major pollen allergen Art v 1 OS=Artemisia vulgaris PE=1	11	7487	0.0E+00
Q2I6J6	Malate dehydrogenase (Fragment) OS=Stevia rebaudiana	119	2193	0.0E+00
B1GV87	NADH dehydrogenase subunit F (Fragment) OS=Hymenol	77	1817	0.0E+00
O04004	Non-specific lipid-transfer protein OS=Ambrosia artemisi	8	100	1.3E+06
K9MJH9	NtPRp27-like (Fragment) OS=Senecio vulgaris PE=4 SV=1	124	3940	0.0E+00
P47919	Nucleoside diphosphate kinase A OS=Flaveria bidentis PE	88	160	4.5E+05
P47920	Nucleoside diphosphate kinase B OS=Flaveria bidentis PE	98	239	5.6E+04
Q96559	Nucleoside diphosphate kinase OS=Helianthus annuus PE	90	238	5.1E+05
A0A076EA72	PawS-like preproalbumin 1 OS=Espeletia schultzii GN=Pa	23	15962	0.0E+00
E1XUL9	Pectate lyase (Fragment) OS=Ambrosia artemisiifolia GN-	12	3	1.3E+06

P27760	Pectate lyase 1 OS=Ambrosia artemisiifolia PE=1 SV=1	2	11	5.2E+05
P27762	Pectate lyase 4 OS=Ambrosia artemisiifolia PE=1 SV=1	16	13	1.0E+06
P27759	Pectate lyase 5 OS=Ambrosia artemisiifolia PE=1 SV=1	5	1	1.2E+06
E1XUL2	Pectate lyase OS=Ambrosia artemisiifolia GN=amba1 PE=	6	2	7.2E+05
E1XUL3	Pectate lyase OS=Ambrosia artemisiifolia GN=amba1.2 PE=	1	10	5.8E+06
E1XUL4	Pectate lyase OS=Ambrosia artemisiifolia GN=amba1.3 PE=	3	4	1.3E+06
E1XUL5	Pectate lyase OS=Ambrosia artemisiifolia GN=amba1.3 PE=	4	5	2.7E+05
E1XUM0	Pectate lyase OS=Ambrosia artemisiifolia GN=amba2.01 PE=	17	14	1.5E+05
A0PJ16	Pectate lyase OS=Artemisia vulgaris PE=2 SV=1	85	1004	0.0E+00
A8CYN7	Peptidyl-prolyl cis-trans isomerase OS=Gerbera hybrida PE=	33	32	3.0E+05
Q94LX7	Phosphoenolpyruvate carboxykinase OS=Flaveria pringlei PE=	139	1127	1.5E+05
A1Y2J9	Phosphoglycerate kinase OS=Helianthus annuus GN=PGK1 PE=	55	59	3.3E+05
I6LNT9	Phosphoglycerate kinase OS=Helianthus annuus GN=PGK2 PE=	54	65	5.6E+04
I6LNU0	Phosphoglycerate kinase OS=Helianthus annuus GN=PGK3 PE=	72	241	2.0E+04
B2KNE6	Phospholipase D OS=Helianthus annuus GN=PLD1 PE=2 SV=1	143	1131	6.6E+04
A9P745	Plastid enolase OS=Helianthus annuus GN=ENO1 PE=2 SV=1	109	1011	4.5E+04
Q6Y8C7	Plastidic Cu/Zn-superoxide dismutase (Fragment) OS=Helianthus	130	893	1.2E+05
Q2KM81	Polcalcin OS=Artemisia vulgaris PE=2 SV=1	74	103	5.2E+05
P00304	Pollen allergen Amb a 3 OS=Ambrosia artemisiifolia var. artemisiifolia	46	117	9.4E+05
P02878	Pollen allergen Amb a 5 OS=Ambrosia artemisiifolia var. artemisiifolia	26	207	8.8E+05
P43174	Pollen allergen Amb p 5a OS=Ambrosia psilostachya PE=1 SV=1	47	373	2.0E+05
Q2KN24	Profilin OS=Ambrosia artemisiifolia PE=2 SV=1	14	43	1.4E+07
Q2KN23	Profilin OS=Ambrosia artemisiifolia PE=2 SV=1	18	45	6.9E+06
Q8H2C9	Profilin-1 OS=Artemisia vulgaris PE=1 SV=3	63	174	2.9E+06
Q64LH0	Profilin-3 OS=Ambrosia artemisiifolia GN=D03 PE=1 SV=1	32	74	5.3E+06
Q1KXH4	Protein TIC 214 OS=Lactuca sativa GN=TIC214 PE=3 SV=1	83	2275	2.5E+05
A0A097NU91	Putative 14-3-3 protein (Fragment) OS=Taraxacum officinale	68	391	9.1E+04
A5HSG4	Putative calmodulin OS=Artemisia annua PE=2 SV=1	27	164	2.5E+05
Q0H284	Putative F1-ATPase alpha subunit (Fragment) OS=Zinnia violacea	122	1016	5.0E+04
Q0H286	Putative glyceraldehyde 3-phosphate dehydrogenase (Fructose 1,6-bisphosphate)	116	211	1.8E+05
A5HSG7	Putative ubiquitin-conjugating enzyme OS=Artemisia annua PE=	62	70	7.3E+05
Q078T1	Putative xyloglucan endotransglucosylase/hydrolase (Fragment)	95	15752	0.0E+00
D4IIH6	Ragweed homologue of Art v 1 OS=Ambrosia artemisiifolia PE=	34	214	2.9E+07
D4IIH5	Ragweed homologue of Art v 1 OS=Ambrosia artemisiifolia PE=	33	219	0.0E+00
D4IIH1	Ragweed homologue of Art v 1 OS=Ambrosia artemisiifolia PE=	32	283	6.9E+06
D3HU71	Ragweed homologue of Art v 1 OS=Ambrosia artemisiifolia PE=	57	284	0.0E+00
A0A0A7E6L1	Rhomboid-like protein (Fragment) OS=Lactuca sativa PE=	113	1037	5.3E+06
R4QUR7	Ribulose-1 5-bisphosphate carboxylase/oxygenase large subunit	19	1018	8.4E+05
A0A076L591	RNA polymerase beta subunit (Fragment) OS=Famatinaria	136	2370	0.0E+00
Q6A199	Superoxide dismutase [Cu-Zn] OS=Helianthus annuus GN=	106	244	9.9E+04
Q41724	TED2 OS=Zinnia violacea PE=2 SV=1	111	1144	1.2E+04
Q3LVE9	TO114-2 (Fragment) OS=Taraxacum officinale GN=To114-2	129	856	4.3E+04
Q3LVQ4	TO23-1 (Fragment) OS=Taraxacum officinale GN=To23-1	105	210	2.3E+05
Q3LVP4	TO38-23 (Fragment) OS=Taraxacum officinale GN=To38-23	128	15963	0.0E+00
A0A0A0QVW1	Mitogen-activated protein kinase kinase kinase 1 plant (Lactuca)	63	16015	0.0E+00
Q3LVN1	TO45-3 (Fragment) OS=Taraxacum officinale GN=To45-3	78	379	8.7E+04
Q3LVJ7	TO65-3 (Fragment) OS=Taraxacum officinale GN=To65-3	137	8091	0.0E+00

P48493	Triosephosphate isomerase cytosolic (Fragment) OS=Lac	50	44	9.3E+05
A0A068EPQ1	Tubulin alpha chain OS=Carthamus tinctorius GN=TUA PE	121	454	3.9E+05
			<u>Total sum</u>	1.0E+08
			<u>Allergen sum</u>	8.7E+07
			%	83

Total sum represents sum of area under extracted ion chromatography (XIC) curve for all confidently identified allergens (APE) by the label free quantification algorithm PEAKS Q. Percentages of allergomes for the respective pollen fractions are calculated by dividing the sum of areas under XIC curve of all officially recognized allergens (here currently 26 allergen entries) with the sum of areas under XIC curve of all pollen fractions and multiplying the result by 100 to obtain percentage. By clicking on the cells E92, F92 and G92, E94, F94 and G94, as well as E95, F95 and G95, you can see the highest value of area under XIC curve among 3 pollen fractions for each allergen.

P) protein extracts of the short ragweed pollen.

lution digested analyses). Each
 genome' share (percentage of
 e Table S5).

SPP Area under XIC curve	APE Area under XIC curve	TOT:SPP:APE (Ratio)	Significance (-10lgP)	Coverage (%)	#Peptides	#Unique
0.0E+00	1.7E+06	0:0:1.00	5.33	1	1	1
1.5E+05	4.1E+04	1.00:1.31:0.36	3.34	2	1	1
5.5E+04	0.0E+00	1.00:0.14:0	14.3	64	17	2
6.6E+04	0.0E+00	1.00:0.14:0	12.77	61	21	3
0.0E+00	0.0E+00	1.00:0:0	8.19	49	17	1
5.4E+04	0.0E+00	0.00:1.87:0	2.22	3	1	1
7.7E+04	0.0E+00	1.00:0.55:0	1.98	26	4	1
2.3E+04	2.5E+05	1.00:0.29:3.15	7.19	27	4	1
0.0E+00	6.5E+05	1.00:0:1.97	4.14	58	6	6
5.6E+04	0.0E+00	1.00:0.39:0	12.5	12	5	5
8.1E+05	0.0E+00	0:1.00:0.34	12.5	2	1	1
2.4E+06	1.2E+07	1.00:2.65:13.95	5.79	7	1	1
8.7E+04	0.0E+00	1.00:1.50:0.43	4.84	1	1	1
0.0E+00	3.9E+03	0:0:1.00	5.45	12	1	1
6.1E+04	5.5E+05	1.00:3.86:35.04	8.46	1	1	1
6.9E+06	1.7E+06	1.00:1.30:0.32	7.54	49	22	22
3.8E+04	2.4E+05	1.00:0.43:2.78	6.68	47	4	4
3.1E+05	0.0E+00	0:1.00:0	11.41	37	5	1
6.3E+05	6.0E+05	1.00:5.03:4.78	8.77	50	7	3
2.4E+04	5.3E+04	1.00:0.03:0.06	10.09	19	7	6
3.4E+04	0.0E+00	1.00:0.47:0	11.89	17	2	2
0.0E+00	0.0E+00	1.00:0.27:0.18	8.46	7	3	3
9.3E+05	8.1E+04	1.00:0.79:0.07	3.19	57	15	8
1.8E+04	0.0E+00	1.00:0.18:0	3.63	81	8	1
4.3E+05	0.0E+00	1.00:1.22:0	18.74	58	16	2
5.3E+04	3.2E+04	1.00:1.20:0.72	2.62	31	12	1
5.4E+03	0.0E+00	1.00:0.54:0	5.24	8	1	1
0.0E+00	2.1E+05	1.00:0:0.85	12.1	15	8	7
0.0E+00	0.0E+00	1.00:0.17:2.04	8.69	3	1	1
3.9E+05	0.0E+00	0:1.00:0	11.09	14	2	1
8.0E+04	5.8E+05	0:0:1.00	6.44	11	2	1
8.1E+04	0.0E+00	0.00:1:0.00	3.12	3	1	1
3.1E+07	1.2E+08	0:1.00:3.97	16.78	72	34	34
0.0E+00	4.7E+05	0:1.00:1.27	0.82	5	2	2
1.8E+05	4.8E+04	1.00:0.39:0.11	11.26	36	6	3
6.4E+04	0.0E+00	1.00:1.16:0	7.61	28	5	1
2.4E+05	1.6E+05	1.00:0.46:0.31	7.79	34	5	2
3.1E+05	3.3E+06	0:1.00:10.74	14.75	3	1	1
1.0E+06	7.2E+05	1.00:0.78:0.54	3.64	77	36	21

8.7E+06	3.8E+05	1.00:16.66:0.73	7.78	88	66	2
1.2E+06	5.1E+05	1.00:1.13:0.49	2.74	83	28	1
1.7E+06	3.5E+05	1.00:1.44:0.29	6.57	87	56	2
5.9E+05	2.8E+05	1.00:0.81:0.39	7.35	87	54	3
4.4E+06	4.6E+06	1.00:0.77:0.81	2.08	88	67	3
1.0E+06	3.3E+05	1.00:0.81:0.26	5.4	88	59	3
2.2E+05	6.0E+04	1.00:0.84:0.22	7.3	88	58	2
1.3E+05	8.3E+04	1.00:0.85:0.56	1.39	83	28	1
3.7E+05	0.0E+00	1.00:5.11:0.12	11.49	8	6	2
2.9E+05	5.1E+05	1.00:0.97:1.69	3.39	81	18	4
0.0E+00	0.0E+00	1.00:0.23:0.06	5.47	1	1	1
1.9E+05	2.3E+05	1.00:0.58:0.70	2.38	29	13	3
2.7E+04	1.7E+05	1.00:0.49:3.01	7.97	36	15	7
0.0E+00	4.9E+04	1.00:0:2.53	3.72	12	7	1
4.6E+04	1.1E+05	1.00:0.69:1.63	2.01	2	1	1
4.2E+04	0.0E+00	1.00:0.95:0	0.78	1	1	1
6.5E+04	0.0E+00	1.00:0.54:0	7.46	44	1	1
1.0E+05	9.2E+05	1.00:0.19:1.75	4.39	41	8	8
2.9E+05	1.3E+07	0:1.00:43.90	11.37	59	14	14
3.4E+06	1.5E+07	0:1.00:4.30	18.02	93	20	10
7.3E+05	8.8E+06	0:1.00:12.12	18.25	55	13	3
8.5E+06	5.8E+06	1.00:0.61:0.41	4.72	99	25	15
4.1E+06	3.1E+06	1.00:0.59:0.46	4.29	83	19	9
0.0E+00	0.0E+00	1.00:0.06:0.29	12.55	28	9	2
1.4E+06	1.9E+06	1.00:0.26:0.35	9.45	62	16	9
2.6E+04	4.3E+06	1.00:0.10:17.43	8.96	0	1	1
0.0E+00	2.3E+05	1.00:0:2.58	8.94	26	8	8
7.4E+04	1.4E+06	1.00:0.30:5.53	11.63	77	18	14
1.7E+04	0.0E+00	1.00:0.34:0	6.06	9	1	1
2.2E+05	2.9E+04	1.00:1.25:0.16	14.77	32	2	1
1.5E+05	4.3E+06	1.00:0.21:5.96	14.73	53	11	11
7.4E+03	3.3E+05	0:1.00:43.85	8.4	8	1	1
1.8E+08	1.4E+07	0:1.00:0.08	17.02	42	19	4
2.7E+07	8.6E+07	0:0.32:1.0	11.02	40	17	3
2.5E+07	0.0E+00	0.28:1:0	13.56	30	10	2
1.1E+07	1.6E+07	0:1.00:1.47	15.06	26	12	4
8.6E+06	0.0E+00	1.00:1.62:0	10.88	4	1	1
2.5E+05	3.3E+06	1.00:0.30:3.90	8.44	5	2	1
1.3E+06	0.0E+00	0:1.00:0.21	16.47	0	1	1
1.1E+05	1.6E+04	1.00:1.09:0.16	8.68	28	4	4
5.4E+04	5.6E+04	1.00:0.74:0.78	1.57	6	2	2
0.0E+00	0.0E+00	1.00:0:0	7.84	7	1	1
6.0E+04	1.8E+05	1.00:0.26:0.75	7	60	4	3
0.0E+00	3.0E+04	0:0:1.00	5.26	5	1	1
0.0E+00	3.5E+04	0:0:1.00	10.00	25.01	1	1
7.1E+04	1.5E+04	1.00:0.81:0.17	1.49	19	2	2
7.8E+05	0.0E+00	0:1.00:0	7.04	6	1	1

8.8E+05	5.5E+05	1.00:0.94:0.59	1.78	69	14	14
0.0E+00	0.0E+00	1.00:0:0	9.55	3	1	1
3.4E+08	3.3E+08					

3.2E+08	3.0E+08					
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94

89

ed and compared proteins within each pollen fraction (TOT, SPP and fractions were calculated by dividing sum of areas under XIC curve of f all proteins for each fraction, separately, and then multiplying with d G95, all these formula can be visualized. Bold faced text denote the or certain protein entry.

Avg. Mass PTM

82152
69527 Deamidation (NQ)
31953 Carbamidomethylation; Oxidation (M); Carbamidomethylation; Oxidation (M); Carbamidomethylation;
41625 Carbamidomethylation; Oxidation (M); Carbamidomethylation; Oxidation (M); Carbamidomethylation;
41712 Carbamidomethylation; Oxidation (M); Carbamidomethylation; Oxidation (M); Carbamidomethylation;
53081
18689 Carbamidomethylation; Deamidation (NQ); Carbamidomethylation; Oxidation (M)
18561 Carbamidomethylation; Deamidation (NQ); Carbamidomethylation; Oxidation (M)
13225
55487
63991 Deamidation (NQ)
11399
60970
9294
77365
43157 Carbamidomethylation; Carbamidomethylation; Oxidation (M); Carbamidomethylation
10524
11897 Deamidation (NQ)
12113 Deamidation (NQ)
49404
17265 Carbamidomethylation
62308
19485 Oxidation (M); Oxidation (M)
10802 Oxidation (M)
36809 Carbamidomethylation; Deamidation (NQ); Oxidation (M)
36918 Deamidation (NQ); Oxidation (M); Oxidation (M)
12663
70854
29079
13404 Carbamidomethylation
19812
33532 Deamidation (NQ)
12789 Carbamidomethylation; Carbamidomethylation; Deamidation (NQ); Oxidation (M); Carbamidomethylat
23005
16136
16200
16217
17354
42311 Carbamidomethylation; Carbamidomethylation; Oxidation (M); Carbamidomethylation

43665 Carbamidomethylation; Carbamidomethylation; Deamidation (NQ); Oxidation (M); Carbamidomethylat
44082 Carbamidomethylation; Deamidation (NQ); Carbamidomethylation; Oxidation (M); Carbamidomethylat
42709 Carbamidomethylation; Carbamidomethylation; Oxidation (M); Carbamidomethylation
42695 Carbamidomethylation; Carbamidomethylation; Oxidation (M); Carbamidomethylation
43637 Carbamidomethylation; Carbamidomethylation; Deamidation (NQ); Oxidation (M); Carbamidomethylat
42913 Carbamidomethylation; Oxidation (M); Carbamidomethylation; Deamidation (NQ); Oxidation (M); 2 mc
42963 Carbamidomethylation; Oxidation (M); Carbamidomethylation; Deamidation (NQ); Oxidation (M); 2 mc
44083 Carbamidomethylation; Deamidation (NQ); Carbamidomethylation; Oxidation (M); Carbamidomethylat
43154 Carbamidomethylation
18129 Carbamidomethylation; Deamidation (NQ); Carbamidomethylation; Oxidation (M); Carbamidomethylat
72880
42303
42408 Carbamidomethylation; Deamidation (NQ)
50144
91916
52027 Deamidation (NQ); Deamidation (NQ)
8157
16694
11375 Carbamidomethylation
4979 Carbamidomethylation; Carbamidomethylation; Carbamidomethylation; Deamidation (NQ)
8710 Carbamidomethylation; Carbamidomethylation; Carbamidomethylation; Deamidation (NQ)
14245 Carbamidomethylation; Oxidation (M); Carbamidomethylation; Deamidation (NQ); Oxidation (M); 2 mc
14100 Carbamidomethylation; Oxidation (M); Carbamidomethylation; Oxidation (M); Carbamidomethylation;
14207 Carbamidomethylation; Carbamidomethylation; Carbamidomethylation
14277 Carbamidomethylation; Oxidation (M); Carbamidomethylation; Oxidation (M); Carbamidomethylation
199811
28873
16848 Oxidation (M); Carbamidomethylation
26751
6321
14643
17243
11896 Carbamidomethylation; Carbamidomethylation; Carbamidomethylation
11304
13260
15566 Carbamidomethylation; Carbamidomethylation; Carbamidomethylation
37307 Deamidation (NQ)
52241 Deamidation (NQ); Oxidation (M)
116578 Carbamidomethylation
15425 Carbamidomethylation
34971
11707
10531
15907
50554
12394
11711 Carbamidomethylation

20540 Carbamidomethylation; Oxidation (M)
49541

2 more
2 more
2 more

tion; Deamidation (NQ)

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Oxidation (M)