Electronic Supplementary Material (ESI) for Analytical Methods.

Verification of exposure to chemical warfare agents through analysis of persistent biomarkers in plants

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A.1. Method optimization and validation

The gradient elution was optimized for each analyte (Table A.1). The chemicals could be analyzed with a single chromatographic method as well, which is the same as described for the A-234 and GB adducts.

Table A. 1. Gradient elution settings for LC-MS/MS analyses. Eluent A is water with 0.2% v/v formic acid and eluent B is ACN with 0.2% v/v formic acid.

Analyte	Eluent A (%)	Linear ramping (min)	Eluent A (%)	Eluent A (%)
A-234-Tyr GB-Tyr MPA-Tyr	100 (hold 1 min)	10	50 (hold 2 min)	100 (hold 3 min)
Cl-Tyr di-Cl-Tyr $^{13}C_6$-Cl-Tyr	100 (hold 2 min)	8	20 (hold 2 min)	100 (hold 3 min)
N1-HETE-His N3-HETE-His	100 (hold 3 min)	3	20 (hold 1 min)	100 (hold 3 min)

For GB-Tyr, linear calibration curves were obtained in the range of 0.05 – 20 ng/mL with R^2 = 0.9997 – 0.99999 (Figure A.1A). The mean values for the quality controls were within 2.6% relative standard deviation at 0.1, 1 and 10 ng/mL (n=10 for each concentration). The stability of the analyte was assessed over two weeks and the concentration was within 15% of the nominal value for 0.1 ng/mL and within 3.3% for 1 and 10 ng/mL.

In addition, linear calibration curves were obtained in the range of 1 – 100 ng/mL with R^2 = 0.9999 – 0.99995 for Cl-Tyr and di-Cl-Tyr as well (Figure A.1B). The mean values for the quality controls were within 20% at 1 ng/mL and within 6% relative standard deviation at both 10 ng/mL and 100 ng/mL (n = 10, for each concentration). The stability of the analytes was assessed over two weeks and the concentration was within 18% of the nominal value for 1 ng/mL and within 3.8% for 10 and 100 ng/mL.

Third, the LC-MS/MS method was validated for N1-HETE-HIS and N3-HETE-HIS. Linear calibration curves were obtained in the range of 1 – 50 ng/mL with R^2 = 9987 – 9997 (Figure A.1C). The mean values of the quality controls were within 5% for 1 and 10 ng/mL N1-HETE-HIS and N3-HETE-HIS (n = 10, for each concentration). The stability of the analytes was assessed over one week and the concentration was within 23% for 1 ng/mL N3-HETE-HIS and within 6% for 1 ng/mL N1-HETE-HIS and 10 mg/mL N1-HETE-HIS and N3-HETE-HIS.

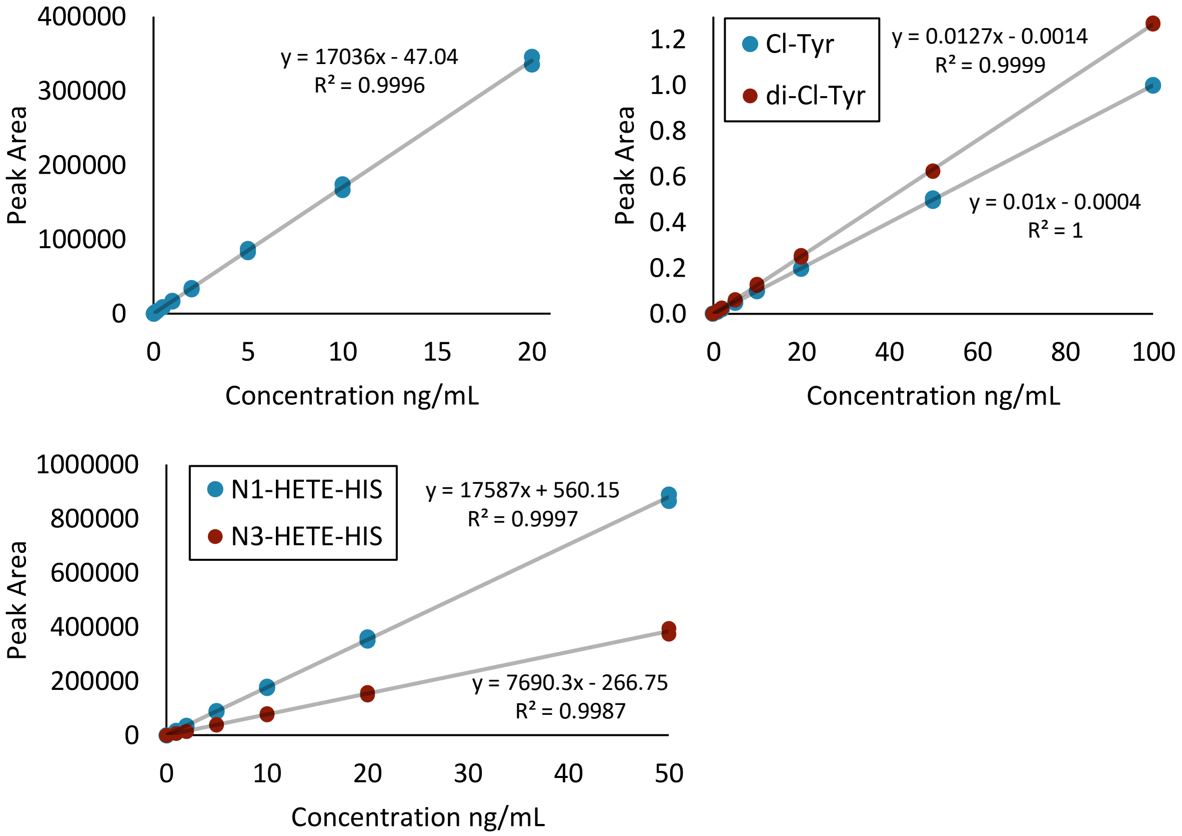

Figure A. 1. Calibration curves analyzed by LC-MS/MS of A) GB-Tyr, B) 3-chlorotyrosine (Cl-Tyr) and 3,5-dichlorotyrosine (di-Cl-Tyr) with internal standard 13C6-3-chloro-L-tyrosine, C) N1-HETE-HIS and N3-HETE-HIS adducts of sulfur mustard.

A.2. Visual examination of vegetation

Figure A. 2. Physical state of nettle leaf upon liquid exposure to A-234.

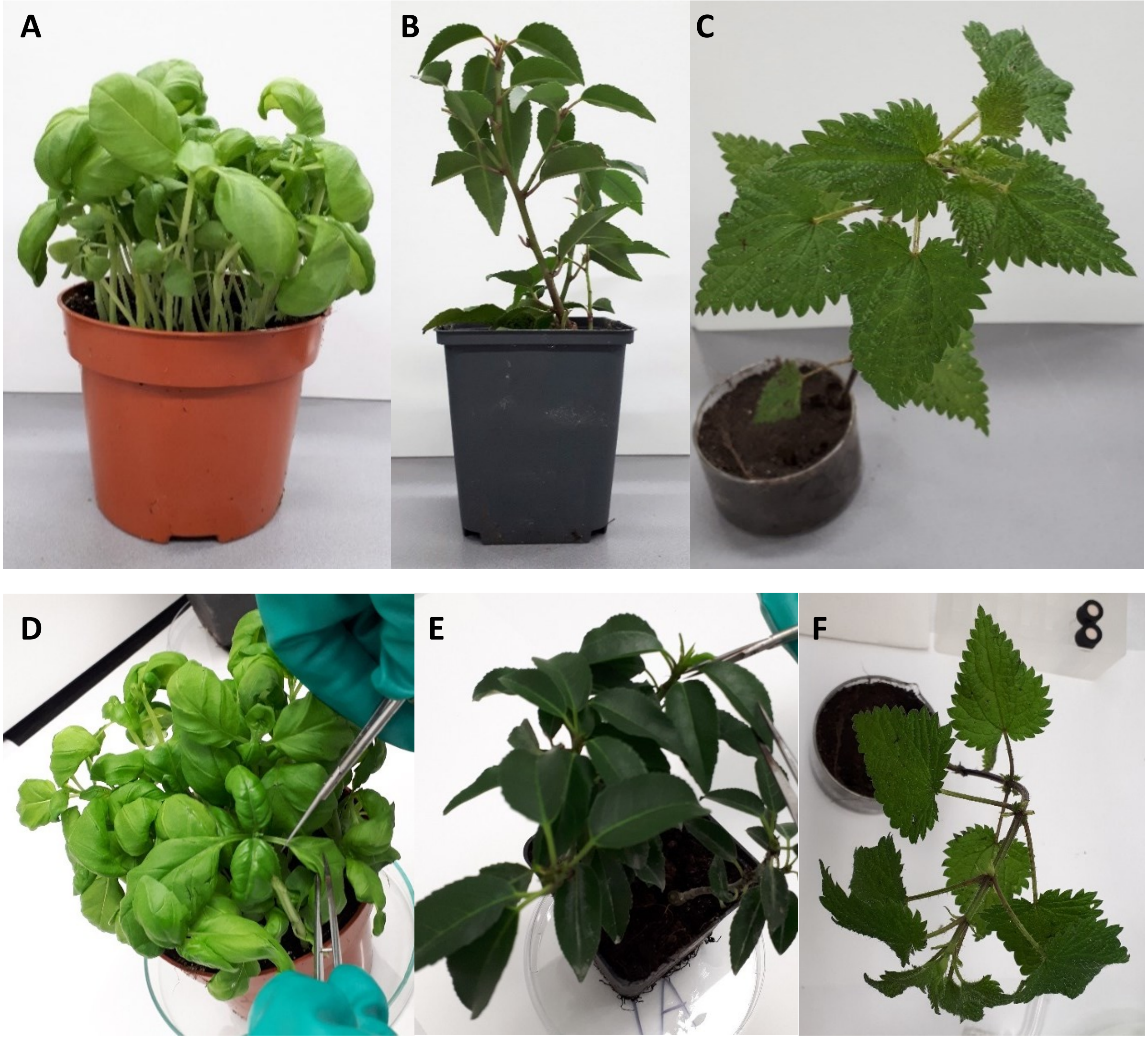

Figure A. 3. No notable differences were observed for A) Laurel, B) Basil and C) Nettle prior to exposure compared to D) Laurel, E) Basil and F) Nettle immediately after vapor exposure of 25 mg/m^3 sarin in the vapor generation set-up.

Figure A. 4. Nettle A) prior to exposure B) after 250 mg/m^3 exposure to sarin. It should be noted that the change could also be due to the dry atmosphere in the vapor generation set-up instead as a result of the chemical warfare agent exposure.

A.3. Chromatograms after three months

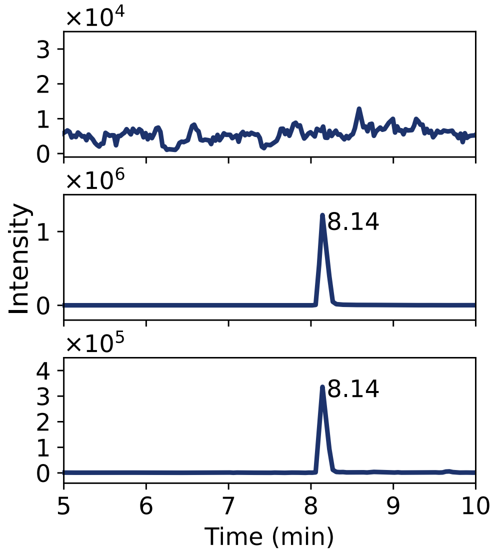

Figure A. 5. Extracted ion chromatograms of phosphylated tyrosine adduct with t_R = 8.14 three months after sarin vapor exposure. A) Sample preparation blank. B) Standard GB-Tyr. C) GB-Tyr measured after plant exposure to 250 mg/m^3 sarin.

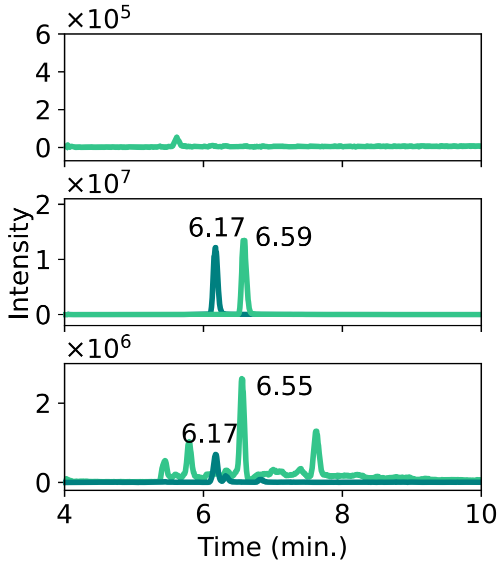

Figure A. 6. Extracted ion chromatograms of chlorinated tyrosine adducts three months after chlorine gas exposure. A) Sample preparation blank. B) Standard Cl-Tyr with t_R = 6.17 min and di-Cl-Tyr with t_R = 6.59 min. C) Cl-Tyr and di-Cl-Tyr after 5 g/m^3 plant exposure.

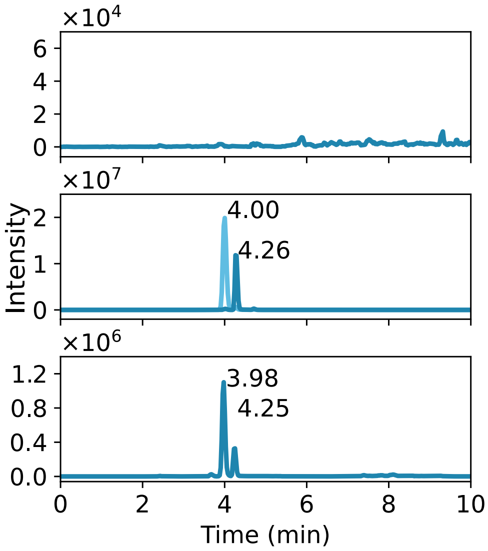

Figure A. 7. Extracted ion chromatograms of N1-HETE-His and N3-HETE-His adducts three months after sulfur mustard vapor exposure. A) Sample preparation blank. B) Standard N1-HETE-His with t_R = 4.00 min and N3-HETE-His with t_R = 4.26 min. C) N1-HETE-His and N3-HETE-His measured after 150 mg/m^3 plant exposure.

Table A. 2. Identified biomarkers in plants after chlorine, sarin or sulfur mustard exposure.

Peptide	**Accession**	**Protein**	**Mass (Da)**	**t_R (min)**	**Exposure**	**Species**	**N (#)[a]**
Y(+120.03)FRLSSLEKCY(+120.03)SR	P93211|14336_SOLLC	14-3-3 protein	1890.9	16.4	GB	Basil	1
KSCSY(+33.96)ELETELSK	P29307|1433_OENEH	14-3-3 protein	1549.7	16.0	Cl	Nettle	1
H(+105.04)DKHELQEAAHNK	P93784|14335_SOLTU	14-3-3 protein	1660.8	20.1	HD	Laurel	1
AEEAAEKY(+120.03)RKPAAAEATAAPPR	P49608|ACOC_CUCMA	Aconitate hydratase, cytoplasmic	2417.2	16.1	GB	Basil	1
CY(+120.03)KLLLPTTLVVADKFAFAEHK	O65396|GCST_ARATH	Aminomethyltransferase, mitochondrial	2626.4	21.2	GB	Laurel	1
GYPGY(+33.96)LYTDLATIYER	B0K8E7|VATB_THEP3	ATP synthase	1927.9	21.3	Cl	Nettle	2
MY(+120.03)Y(+120.03)EAKETLELAEAVKR	Q0ZJ14|ATPE_VITVI	ATP synthase, chloroplastic	2283.1	21.6	GB	Laurel	1
QMLPLCH(+105.04)CQTLELAEAGGLR	Q2MI94|ATPE_SOLLC	ATP synthase, chloroplastic	2287.1	21.6	HD	Basil	1
EAQAVADDVFSLFISEEVDKVELLY(+33.96)TK	Q01908|ATPG1_ARATH	ATP synthase, chloroplastic	3091.5	22.8	Cl	Nettle	2
WEHY(+120.03)FMESLASELAAR	P29790|ATPG_TOBAC	ATP synthase, chloroplastic	2058.9	20.2	GB	Laurel	1
KVEY(+120.03)MRVLMGDGLFLQEGSWK	A6MM21|ATPA_BUXMI	ATP synthase, chloroplastic	2605.3	22.0	GB	Basil	1
NY(+120.03)MQVDPFQESGVLNEENLAESK	Q68RZ9|ATPB_PANGI	ATP synthase, chloroplastic	2760.2	18.8	GB	Basil	1
Y(+120.03)FKLATSGSGVSTLEK	Q68RZ9|ATPB_PANGI	ATP synthase, chloroplastic	1806.9	17.1	GB	Basil	1
Y(+120.03)VGPAVDPLDSTPNAVMPR	Q68RZ9|ATPB_PANGI	ATP synthase, chloroplastic	2118.0	20.8	GB	Basil	1
RY(+120.03)PAVDPLDSFHVVMPR	Q85V35|ATPB_LACPU	ATP synthase, chloroplastic	2118.0	20.7	GB	Basil	1
VGLTALTIAEY(+33.96)FR	O03081|ATPB_PSINU	ATP synthase, chloroplastic	1486.8	21.2	Cl	Nettle	2
VGLTALTIAEY(+67.92)FR	O03081|ATPB_PSINU	ATP synthase, chloroplastic	1520.7	21.6	Cl	Nettle	1
QVY(+120.03)HLNEQNLAESK	Q2L917|ATPB_GOSHI	ATP synthase, chloroplastic	1791.9	16.6	GB	Laurel	1
Y(+120.03)NMCY(+120.03)RWWRLNEKNLAESK	Q2L917|ATPB_GOSHI	ATP synthase, chloroplastic	2743.3	19.9	GB	Laurel	1
Y(+120.03)Y(+120.03)Y(+120.03)VVLSTEMGTLKER	Q2L917|ATPB_GOSHI	ATP synthase, chloroplastic	2311.1	20.1	GB	Laurel	1
KYY(+120.03)NMY(+120.03)SPAGYLENK	P19023|ATPBM_MAIZE	ATP synthase, mitochondrial	2079.9	19.8	GB	Basil	1
Y(+120.03)DADSGGVVLYVK	Q41396|VATE_SPIOL	ATPase	1504.7	18.5	GB	Basil	1
AY(+120.03)ENGTLSVAGR	O80860|FTSH2_ARATH	ATP-dependent zinc metalloprotease, chloroplastic	1356.6	23.1	GB	Basil	1
EALGKAELKEALASLEH(+105.04)KEETLK	Q655S1|FTSH2_ORYSJ	ATP-dependent zinc metalloprotease, chloroplastic	2641.4	20.3	HD	Basil	1
Y(+33.96)AGVGAAIEYAVLHLK	P42737|BCA2_ARATH	Carbonic anhydrase, chloroplastic	1707.9	20.9	Cl	Nettle	2
WY(+120.03)WY(+120.03)KLLSSVDLLEEKLR	B9N843|ACCC2_POPTR	Biotin carboxylase, chloroplastic	2580.3	21.0	GB	Basil	1
H(+105.04)NLTDDQLSEFK	Q39752|CALM_FAGSY	Calmodulin	1550.7	21.4	HD	Laurel	2
GPILLEDY(+33.96)HLVEK	P48350|CATA1_CUCPE	Catalase	1558.8	20.7	Cl	Nettle	1

LPACCAY(+120.03)RLLEKENNK	P48350|CATA1_CUCPE	Catalase	1984.0	16.0	GB	Laurel	1
Y(+120.03)FELEQENNKNVASSTGK	P48350|CATA1_CUCPE	Catalase	2177.0	15.9	GB	Basil	1
GPLENLADHLADPVNNNAWAY(+33.96)ATKLCPGK	P09755|CB22_SOYBN	Chlorophyll binding protein, chloroplastic	3125.5	22.3	Cl	Nettle	2
CY(+120.03)GDYLGNPNLLVVPK	P09756|CB23_SOYBN	Chlorophyll binding protein, chloroplastic	1883.9	20.5	GB	Laurel	1
GY(+120.03)CDYLGNPSLVVPAR	P09756|CB23_SOYBN	Chlorophyll binding protein, chloroplastic	1842.9	20.2	GB	Laurel	1
LVY(+120.03)FYLAPELLGK	P27522|CB13_SOLLC	Chlorophyll binding protein, chloroplastic	1644.9	21.6	GB	Basil	1
DHVKPVSSGSY(+120.03)YGDPR	P04783|CB25_PETSP	Chlorophyll binding protein, chloroplastic	1882.9	19.0	GB	Basil	1
Y(+120.03)Y(+120.03)PNATGDKGYPGGK	P36494|CB4_SPIOL	Chlorophyll binding protein, chloroplastic	1826.8	17.8	GB	Basil	1
KLY(+120.03)RYLKFDLDSLDQNLAK	Q07473|CB4A_ARATH	Chlorophyll binding protein, chloroplastic	2462.3	22.3	GB	Basil	1
NY(+120.03)WELLHGR	Q07473|CB4A_ARATH	Chlorophyll binding protein, chloroplastic	1306.6	17.8	GB	Basil	1
Y(+120.03)CMVQSTPFQDHRSQVLVLR	Q07473|CB4A_ARATH	Chlorophyll binding protein, chloroplastic	2526.2	21.8	GB	Laurel	1
Y(+120.03)GELLHGR	Q07473|CB4A_ARATH	Chlorophyll binding protein, chloroplastic	1306.6	17.8	GB	Basil	2
Y(+120.03)YHELLHGR	Q07473|CB4A_ARATH	Chlorophyll binding protein, chloroplastic	1306.6	18.0	GB	Basil	1
EFLVLH(+105.04)LQFELDSLDQGGLAK	Q9XF88|CB4B_ARATH	Chlorophyll binding protein, chloroplastic	2476.3	22.3	HD	Basil	2
EVPYLH(+105.04)LQFDLDSLDQNLAK	Q9XF88|CB4B_ARATH	Chlorophyll binding protein, chloroplastic	2462.2	22.1	HD	Basil	2
H(+105.04)GVFLWSWFH(+105.04)WFDNCAGLSADEPTFAK	P08221|CB21_CUCSA	Chlorophyll binding protein, chloroplastic	3377.5	22.0	HD	Basil	1
Y(+120.03)GCDYLGNPSLVVPAR	Q10HD0|CB23_ORYSJ	Chlorophyll binding protein, chloroplastic	1842.9	20.4	GB	Basil	1
RY(+33.96)VVDDAGVLSR	P29357|HSP7E_SPIOL	Chloroplast envelope membrane	1382.7	17.4	Cl	Nettle	1
KLLRY(+120.03)LPGESDSDFSDFSSK	Q9SA52|CP41B_ARATH	Chloroplast stem-loop binding protein, chloroplastic	2410.1	19.2	GB	Laurel	1
KQPLAQKLY(+120.03)SDSDFSDFSSK	Q9SA52|CP41B_ARATH	Chloroplast stem-loop binding protein, chloroplastic	2410.1	19.5	GB	Basil	1
RY(+120.03)LLKLPGESDSDFSDFSSK	Q9SA52|CP41B_ARATH	Chloroplast stem-loop binding protein, chloroplastic	2410.1	19.5	GB	Basil	1
Y(+120.03)Y(+120.03)LLDVVYDLNGR	Q9SA52|CP41B_ARATH	Chloroplast stem-loop binding protein, chloroplastic	1841.9	21.8	GB	Basil	1
VAVEAQWVADY(+120.03)AVK	Q0WLB5|CLAH2_ARATH	Clathrin	1667.8	17.8	GB	Basil	1
TPLTDAAAAY(+120.03)YRR	P25076|CY11_SOLTU	Cytochrome	1587.8	19.7	GB	Laurel	1
H(+105.04)HLTFPLLSPDPTTK	A6MMV7|CYF_ILLOL	Cytochrome	1807.9	21.8	HD	Basil	2
QFY(+120.03)SVTVESAEATLK	Q9SRZ6|ICDHC_ARATH	Cytosolic isocitrate dehydrogenase [NADP]	1791.9	18.5	GB	Laurel	1
GFVY(+120.03)DLLLLPR	F4JLP5|PLPD2_ARATH	Dihydrolipoyl dehydrogenase, chloroplastic	1424.8	22.8	GB	Basil	1
KYH(+105.04)VAEMNKR	P34824|EF1A1_HORVU	Elongation factor	1379.7	15.3	HD	Laurel	1

LPLQDVY(+33.96)K	Q03033|EF1A_WHEAT	Elongation factor	1008.5	19.7	Cl	Nettle	1
DY(+120.03)LPGHKKLTLTR	O24310|EFTU_PEA	Elongation factor, chloroplastic	1660.9	19.8	GB	Basil	1
KWSY(+120.03)LFAVEDVFSLTGR	Q43467|EFTU1_SOYBN	Elongation factor, chloroplastic	2137.1	23.4	GB	Basil	1
H(+105.04)LEAPSRLLAAQPK	Q6ZA06|GUN20_ORYSJ	Endoglucanase	1634.9	20.1	HD	Laurel	1
ATLPAFY(+67.92)LKKLPLPLR	Q42971|ENO_ORYSJ	Enolase	1908.1	21.7	Cl	Nettle	1
KNEVHKY(+120.03)RDDTLLADEELAK	P56337|IF5A5_SOLTU	Eukaryotic translation initiation factor	2506.2	20.3	GB	Basil	1
WPY(+120.03)Y(+120.03)LFDLFDDWLR	P23225|GLTB_MAIZE	Ferredoxin-dependent glutamate synthase, chloroplastic	2188.0	22.3	GB	Basil	1
NGY(+120.03)LSFLANLVLSDR	Q43155|GLTB_SPIOL	Ferredoxin-dependent glutamate synthase, chloroplastic	1800.9	21.0	GB	Basil	1
Y(+120.03)VMAAEKPAAADAPAAEPK	Q69RJ0|GLTB_ORYSJ	Ferredoxin-dependent glutamate synthase, chloroplastic	2020.0	17.7	GB	Basil	1
VVPLLEAY(+67.92)VPK	Q69RJ0|GLTB_ORYSJ	Ferredoxin-dependent glutamate synthase, chloroplastic	1294.6	20.5	Cl	Nettle	1
H(+105.04)DLLQLSGHDGGTGASPVSSLK	Q43155|GLTB_SPIOL	Ferredoxin-dependent glutamate synthase, chloroplastic	2280.1	18.7	HD	Basil	1
TY(+120.03)SNTGVKGAVNVQWDKK	P25851|F16P1_ARATH	Fructose-1,6-bisphosphatase, chloroplastic	2114.1	19.1	GB	Laurel	1
H(+105.04)DELVLFVEHR	P46256|ALF1_PEA	Fructose-bisphosphate aldolase, cytoplasmic	1497.8	21.5	HD	Laurel	1
WKYWY(+120.03)VLKENNVLPGLK	P46256|ALF1_PEA	Fructose-bisphosphate aldolase, cytoplasmic	2269.2	21.3	GB	Basil	1
QECKH(+105.04)TDVLQENNVLPGLK	O65581|ALFC5_ARATH	Fructose-bisphosphate aldolase, cytosolic	2269.1	20.9	HD	Basil	1
RPLTY(+33.96)GLLLASLGLEWDNGGR	P16096|ALFC_SPIOL	Fructose-bisphosphate aldolase, cytosolic	2334.2	18.4	Cl	Nettle	1
Y(+120.03)Y(+120.03)LVFEVLQK	Q9XQ94|GLNA2_MEDSA	Glutamine synthetase leaf isozyme, chloroplastic	1540.8	15.8	GB	Basil	1
H(+105.04)KLLNLDVTPYTDK	O22506|GLNA2_DAUCA	Glutamine synthetase, chloroplastic	1760.9	21.3	HD	Basil	1
HPY(+120.03)LSAYGEDGKR	O22506|GLNA2_DAUCA	Glutamine synthetase, chloroplastic	1611.7	15.1	GB	Basil	1
QMY(+120.03)HVFEVLQK	O22506|GLNA2_DAUCA	Glutamine synthetase, chloroplastic	1540.8	15.9	GB	Basil	1
RY(+120.03)WTPKGEGNER	O22506|GLNA2_DAUCA	Glutamine synthetase, chloroplastic	1611.8	15.1	GB	Laurel	1
KHKY(+67.92)WDELFGGYLYFHK	O24338|ASNS_SANAU	Glutamine-dependent asparagine synthetase	2298.0	21.0	Cl	Nettle	1
Y(+120.03)LVRHYPLDVVVDFMR	P09044|G3PB_TOBAC	Glyceraldehyde-3-phosphate dehydrogenase B, chloroplastic	2141.1	22.9	GB	Basil	1
HSMLGTFY(+120.03)ER	P09044|G3PB_TOBAC	Glyceraldehyde-3-phosphate, chloroplastic	1359.6	15.8	GB	Basil	1
LTLFGDKPVAVY(+33.96)GPR	P08735|G3PC1_MAIZE	Glyceraldehyde-3-phosphate, cytosolic	1665.9	22.1	Cl	Nettle	1
KGADVCH(+105.04)VVEAVR	O49954|GCSP_SOLTU	Glycine decarboxylase	1486.8	16.2	HD	Basil	1
WQQAAEKY(+120.03)RQPAAAEATAPVPK	P26969|GCSP_PEA	Glycine dehydrogenase, mitochondrial	2530.3	17.3	GB	Basil	1

Y(+33.96)AASDLRKAK	Q01899|HSP7M_PHAVU	Heat shock protein, mitochondrial	1155.6	17.3	Cl	Nettle	1
MSY(+120.03)AFFADYTEAHLK	Q9FE01|APX2_ORYSJ	L-ascorbate peroxidase, cytosolic	1912.8	20.6	GB	Basil	1
LAEEAAEKRY(+120.03)KPAAAEDGVPAPK	P30184|AMPL1_ARATH	Leucine aminopeptidase	2530.3	17.1	GB	Laurel	1
GY(+120.03)KLEGDGGPGTLKK	O24248|PRU1_PRUAV	Major allergen Pru av 1	1638.8	15.7	GB	Laurel	1
H(+105.04)PELEGDGGPGTLK	O24248|PRU1_PRUAV	Major allergen Pru av 2	1510.7	16.4	HD	Basil	1
KRQQY(+120.03)VCTSELPPPR	O24248|PRU1_PRUAV	Major allergen Pru av 3	1921.0	21.2	GB	Laurel	1
LYY(+120.03)Y(+120.03)VLRFESLKPSDTDLGSK	O49079|PSBO_FRIAG	Oxygen-evolving enhancer, chloroplastic	2733.3	21.0	GB	Basil	1
LSEEELGKGH(+105.04)AK	P14226|PSBO_PEA	Oxygen-evolving enhancer, chloroplastic	1401.7	15.5	HD	Basil	1
H(+105.04)EGPLEVSVLKDR	P85194|PSBO_HELAN	Oxygen-evolving enhancer, chloroplastic	1582.8	20.0	HD	Laurel	1
SEQWNVEVY	Q40459|PSBO_TOBAC	Oxygen-evolving enhancer, chloroplastic	1595.7	18.9	Cl	Nettle	1
H(+105.04)GENWLEYPGQVLR	P16059|PSBP_PEA	Oxygen-evolving enhancer, chloroplastic	1801.9	20.8	HD	Basil	1
Y(+120.03)MQWLEYPGQVLR	P16059|PSBP_PEA	Oxygen-evolving enhancer, chloroplastic	1801.9	21.1	GB	Basil	1
Y(+120.03)WWWEYPGKVLR	P85189|PSBP_HELAN	Oxygen-evolving enhancer, chloroplastic	1801.9	21.0	GB	Laurel	1
DGDATEH(+105.04)HKLLSATVNDGK	Q04127|PSBP3_TOBAC	Oxygen-evolving enhancer, chloroplastic	2112.0	16.4	HD	Basil	1
EAVH(+105.04)AH(+105.04)APSDELEYPGQVLR	Q04127|PSBP3_TOBAC	Oxygen-evolving enhancer, chloroplastic	2427.2	20.3	HD	Basil	1
SY(+120.03)NDELEYPGKVLR	Q04127|PSBP3_TOBAC	Oxygen-evolving enhancer, chloroplastic	1801.9	21.2	GB	Basil	1
Y(+120.03)CVTPNVVVAADNAAPPR	P83218|PME_DAUCA	Pectinesterase	1976.0	20.1	GB	Laurel	1
Y(+120.03)TWASLAAEAKK	O49006|PME3_ARATH	Pectinesterase	1457.7	18.8	GB	Laurel	1
HVVFGQVVEPY(+33.96)GLPK	Q39613|CYPH_CATRO	Peptidyl-prolyl cis-trans isomerase	1701.9	19.1	Cl	Nettle	1
QLVNY(+120.03)VGTEAVAK	P50318|PGKH2_ARATH	Phosphoglycerate kinase, chloroplastic	1510.8	18.4	GB	Laurel	1
REVLLPTTLVVADKFAY(+120.03)NSK	P41758|PGKH_CHLRE	Phosphoglycerate kinase, chloroplastic	2383.3	22.0	GB	Basil	1
HY(+120.03)VFAVGTEAVAK	Q42961|PGKH_TOBAC	Phosphoglycerate kinase, chloroplastic	1510.8	18.7	GB	Basil	1
H(+105.04)ELAGFQYLGGPETGEK	P0DKC3|PGP1A_ARATH	Phosphoglycolate phosphatase, chloroplastic	1936.9	22.0	HD	Laurel	1
H(+105.04)MQEPLVVGALK	P0DKC3|PGP1A_ARATH	Phosphoglycolate phosphatase, chloroplastic	1425.8	17.4	HD	Laurel	1
KFY(+120.03)Y(+120.03)DGTGLFQTLVGLK	P26302|KPPR_WHEAT	Phosphoribulokinase, chloroplastic	2189.1	22.3	GB	Basil	1
WLYGY(+33.96)CPYYHVSVLEFDGQFDR	P26302|KPPR_WHEAT	Phosphoribulokinase, chloroplastic	2790.2	22.0	Cl	Nettle	1
WH(+105.04)EPAYPGGPLFNPLGFGK	Q9SY97|LHCA3_ARATH	Photosystem chlorophyll binding protein, chloroplastic	2188.1	22.2	HD	Basil	1
KHY(+120.03)WALAPELLGK	Q9SY97|LHCA3_ARATH	Photosystem chlorophyll binding protein, chloroplastic	1644.9	21.7	GB	Basil	1
KTY(+120.03)HPLVYDTWESPK	P12372|PSAD_SOLLC	Photosystem I reaction center, chloroplastic	1983.0	20.3	GB	Laurel	1
RRNNVTEALH(+105.04)TYH(+105.04)YFYWPLFGGSTGGLLR	P36213|PSAD_HORVU	Photosystem I reaction center, chloroplastic	3634.8	22.3	HD	Basil	1

Y(+120.03)AHPADGLPHLLVSTAQR	P13192|PSAF_HORVU	Photosystem I reaction center, chloroplastic	2065.1	21.4	GB	Basil	1
AAEEAAEKY(+120.03)RKPAAAEATPVAPK	P12354|PSAE_SPIOL	Photosystem I reaction center, chloroplastic	2488.3	16.1	GB	Laurel	1
WSFAAEH(+105.04)HPENLLFPEEVLPR	Q2MIA5|PSBD_SOLLC	Photosystem II D2	2622.3	20.5	HD	Basil	2
AAEDPEFETFY(+33.96)TK	Q3MA59|PSBD_TRIV2	Photosystem II D2	3877.4	20.7	Cl	Nettle	1
WKY(+120.03)VY(+120.03)Y(+120.03)PKSVGRATELNAVNYVSPR	P0C367|PSBC_ORYSJ	Photosystem II reaction center	3319.6	21.1	GB	Basil	1
Y(+120.03)AEDGTLALAGR	Q09G50|PSBC_PLAOC	Photosystem II reaction center	1355.6	23.6	GB	Laurel	1
QRDLWHAPY(+67.92)KVLVGGVATELNAVNYVSPR	Q09G50|PSBC_PLAOC	Photosystem II reaction center	3319.6	21.0	Cl	Nettle	1
QSFDH(+105.04)TLAVGWLGHPLFR	P56777|PSBB_ARATH	Photosystem II reaction center	2185.1	21.1	HD	Basil	1
LMVVY(+33.96)ERTFPVVLVDGDGLVR	Q06FP2|PSBB_PELHO	Photosystem II reaction center	2410.2	22.5	Cl	Nettle	1
VPVY(+33.96)FETFPVVLVDGDGLVR	Q06FP2|PSBB_PELHO	Photosystem II reaction center	2254.1	22.7	Cl	Nettle	1
FVDPSDPLLDFY(+120.03)R	Q70XY1|PSBB_AMBTC	Photosystem II reaction center	1702.8	22.1	GB	Basil	1
GY(+120.03)HLGDGNAVGWLGHPLFR	P56777|PSBB_ARATH	Photosystem II reaction center	2185.1	21.5	GB	Basil	1
VFDPSDPLLDFY(+120.03)R	P56777|PSBB_ARATH	Photosystem II reaction center	1702.8	22.1	GB	Basil	1
RY(+120.03)FGKVEDEDFVEFAGVDVSK	P11970|PLAS2_POPNI	Plastocyanin B, chloroplastic	2555.2	20.1	GB	Laurel	1
ERPY(+33.96)EFMLNAPGEVYSVTLSEK	P00288|PLAS_VICFA	Plastocyanin	2592.2	21.4	Cl	Nettle	1
GPEVY(+33.96)PMYLNAPGEVYSVTLSEK	P00288|PLAS_VICFA	Plastocyanin	2576.2	21.3	Cl	Nettle	1
KVY(+120.03)VSY(+120.03)VVFDEDEVPARDVAK	P07030|PLAS_SILLB	Plastocyanin, chloroplastic	2667.3	19.3	GB	Laurel	1
Y(+120.03)CMTQDQEGVVPEMTVPK	Q9FHQ6|UBQ9_ARATH	Polyubiquitin	2173.9	20.4	GB	Laurel	1
LEGAYDRY(+33.96)FQLEAASQQFNGYELDGR	Q9LJL3|PREP1_ARATH	Presequence protease 1, chloroplastic/mitochondrial	3073.4	22.2	Cl	Nettle	1
VVAEAAKAQFSNKAY(+120.03)YDK	Q2JRU4|AMPA_SYNJA	Probable cytosol aminopeptidase	2122.0	17.4	GB	Laurel	1
Y(+120.03)RKMVMGLDKSLEAEFLDR	P83344|XYNB_PRUPE	Putative beta-D-xylosidase	2420.2	22.8	GB	Laurel	1
Y(+120.03)TLPGHKKAFLPR	P83344|XYNB_PRUPE	Putative beta-D-xylosidase	1646.9	18.6	GB	Laurel	2
Y(+120.03)HNHY(+120.03)LLVGQLEWR	P31414|AVP1_ARATH	Pyrophosphate-energized vacuolar membrane proton pump	2067.0	16.5	GB	Basil	1
MCVVY(+120.03)DLTDPFGLLTLDHK	Q40521|RB11B_TOBAC	Ras-related protein Rab11B	2299.1	21.9	GB	Basil	1
RRKRY(+120.03)YVELSEVLYNR	P28644|ROC1_SPIOL	ribonucleoprotein, chloroplastic	2263.2	22.6	GB	Basil	1
RY(+120.03)KDEAAPAKRPAEAPK	Q4FP12|RS16_PELUB	ribosomal protein	2017.1	15.8	GB	Basil	1
RKY(+120.03)ADAPAEAPK	O22518|RSSA_SOYBN	ribosomal protein	1435.7	15.7	GB	Basil	1
TPKFLEGGSVY(+120.03)ELVEK	Q4FG71|RR3_RANMC	ribosomal protein, chloroplastic	1915.0	19.6	GB	Laurel	1
AEERDKY(+120.03)RKPAAAEAPAEAPK	P24929|RK12_TOBAC	ribosomal protein, chloroplastic	2417.2	16.1	GB	Basil	1
VAY(+33.96)PIDLFEEGSVTNLFTSIVGNVFGFK	P48711|RBL_PICAB	RuBisCO	3096.5	23.0	Cl	Nettle	2

GHYLNATAATC(+67.92)EEMLKR	Q1KVV0|RBL_TETOB	RuBisCO	1974.8	16.2	Cl	Nettle	2
DY(+120.03)MEVHSGTVVGK	P19163|RBL_NEUMU	RuBisCO	1540.7	15.1	GB	Basil	1
EY(+120.03)FDPSGTVVGK	P19163|RBL_NEUMU	RuBisCO	1417.7	15.6	GB	Basil	1
MVENY(+120.03)KY(+120.03)Y(+120.03)DDENVNSKPFMR	P19163|RBL_NEUMU	RuBisCO	2901.2	19.0	GB	Basil	1
MWY(+120.03)VHSGTVVGQLEWR	P19163|RBL_NEUMU	RuBisCO	2067.0	16.5	GB	Basil	1
TY(+120.03)WTKDDENVNSQPETR	P19163|RBL_NEUMU	RuBisCO	2202.0	20.3	GB	Basil	1
WY(+120.03)MVHSGTVVGQLEWR	P19163|RBL_NEUMU	RuBisCO	2067.0	16.5	GB	Basil	2
WY(+120.03)PDHSGTVVGKLEWR	P19163|RBL_NEUMU	RuBisCO	2049.0	16.5	GB	Basil	1
NNAAQSH(+105.04)KWDLAAEGANLLR	P28420|RBL_UNCGR	RuBisCO	2283.1	19.2	HD	Basil	1
LTYYTPEY(+33.96)NPKDTDILAAFR	P28438|RBL_PASQU	RuBisCO	2424.1	22.5	Cl	Nettle	1
LTYYTPEY(+33.96)ETK	P48706|RBL_LACSA	RuBisCO	1440.6	19.4	Cl	Nettle	2
MAVWTKH(+105.04)WYRSDVWTDGLTSLDR	Q33438|RBL_ERYCG	RuBisCO	2927.4	20.6	HD	Basil	1
AVYY(+120.03)FLTAGREDDKTFDANSQPFMR	P19163|RBL_NEUMU	RuBisCO	3061.4	20.5	GB	Laurel	1
WY(+120.03)Y(+120.03)SGVNVVNSQPFMR	P19163|RBL_NEUMU	RuBisCO	2186.0	20.9	GB	Laurel	1
DEDNVNSQPFY(+33.96)DPK	P19163|RBL_NEUMU	RuBisCO	1700.7	18.9	Cl	Nettle	1
EAAATDAEALY(+33.96)K	P19163|RBL_NEUMU	RuBisCO	1285.6	22.7	Cl	Nettle	1
EEENVNSKPY(+33.96)PR	P19163|RBL_NEUMU	RuBisCO	1494.7	18.6	Cl	Nettle	1
Y(+67.92)TSASGLHAGTVVGK	P19163|RBL_NEUMU	RuBisCO	1514.7	15.7	Cl	Nettle	1
RY(+120.03)MDTDLLAAFR	P48708|RBL_MOROL	RuBisCO	1590.8	21.7	GB	Laurel	1
WY(+120.03)DHTAGAVEEMLKR	Q32303|RBL_GALLU	RuBisCO	1924.9	17.8	GB	Basil	1
Y(+120.03)HLLEQDR	Q33438|RBL_ERYCG	RuBisCO	1192.6	17.0	GB	Basil	1
GYY(+120.03)LADAASKEDLKAR	P21239|RUB1_BRANA	RuBisCO	1889.9	18.6	GB	Laurel	1
KKDCY(+120.03)RLLEELEQK	P34794|RUB2_BRANA	RuBisCO	1914.0	21.5	GB	Basil	1
KVY(+33.96)LSFLAYKFKDYR	P19310|RBS4_LEMGI	RuBisCO	1974.0	19.9	Cl	Nettle	1
H(+105.04)ELSEESLKEGK	Q08185|RBS5_MESCR	RuBisCO	1489.7	16.4	HD	Laurel	1
WRWY(+120.03)DVSDDKKDLAR	O98997|RCA_VIGRR	RuBisCO activase	2072.0	19.9	GB	Laurel	1
H(+105.04)WDYMLVQEQENVK	Q01587|RCA_CUCSA	RuBisCO activase	1922.9	21.4	HD	Basil	1
Y(+120.03)NDEDKKTVDAATPK	Q40281|RCA_MALDO	RuBisCO activase	1813.8	17.7	GB	Laurel	1
LY(+33.96)SEAALGDANQDLAK	Q40281|RCA_MALDO	RuBisCO activase	1711.8	19.5	Cl	Nettle	1
CY(+120.03)PEDPTAEGFYLAPAFFDK	Q7X9A0|RCA1_LARTR	RuBisCO activase	2400.0	21.9	GB	Basil	1
RY(+120.03)Y(+120.03)FLVQEQERGRK	Q7X9A0|RCA1_LARTR	RuBisCO activase	2111.0	19.3	GB	Basil	1

Y(+120.03)AQVGKCLVQEQENVK	Q7X9A0|RCA1_LARTR	RuBisCO activase	1955.0	20.0	GB	Basil	1
Y(+120.03)TNTDRWNLLEDVSDDQKDLAR	Q7X9A0|RCA1_LARTR	RuBisCO activase	2786.3	20.9	GB	Basil	1
H(+105.04)GNLEDVSDDKQDLAR	Q7X999|RCA2_LARTR	RuBisCO activase	1915.9	20.9	HD	Laurel	1
KLVAVY(+33.96)DLSLNENANGLAR	A9P822|METK1_POPTR	S-adenosylmethionine	2093.1	19.3	Cl	Nettle	1
TADY(+67.92)RRHKLLSATVK	P09439|LOX2_SOYBN	Seed linoleate 9S-lipoxygenase-2	1825.9	16.4	Cl	Nettle	1
SSAKVAEY(+120.03)VKAK	Q94C74|GLYM2_ARATH	Serine hydroxymethyltransferase, mitochondrial	1399.7	16.0	GB	Basil	1
LDESTGYIDY(+33.96)DQLEK	P50433|GLYM_SOLTU	Serine hydroxymethyltransferase, mitochondrial	1821.8	18.7	Cl	Nettle	1
CPEAAEKY(+120.03)RKPAAAEATVPAPK	Q940H6|SRK2E_ARATH	Serine/threonine-protein kinase	2417.2	16.1	GB	Basil	1
RDEAAEKY(+120.03)RQPAAAEATVPAPK	Q940H6|SRK2E_ARATH	Serine/threonine-protein kinase	2488.2	16.2	GB	Basil	1
Y(+33.96)NLSLGLGLNK	P84187|SGAT_MAIZE	Serine--glyoxylate aminotransferase	1224.6	18.9	Cl	Nettle	2
H(+105.04)DVYMWVVATANLLEESTPTVDGK	Q9THX6|TL29_SOLLC	Thylakoid lumenal, chloroplastic	2779.3	22.2	HD	Basil	1
KNQY(+120.03)LEAEWNAK	O20250|TKTC_SPIOL	Transketolase, chloroplastic	1612.8	17.8	GB	Laurel	2
YPRY(+120.03)NWTAGSYK	O20250|TKTC_SPIOL	Transketolase, chloroplastic	1624.7	16.0	GB	Basil	1
KHLNYMAAKSHNY(+33.96)LLLGTGSELELAAK	Q8RWV0|TKTC1_ARATH	Transketolase, chloroplastic	3005.5	20.9	Cl	Nettle	1
SPEEAAEKY(+120.03)RKPAAAEATAVPPK	F4IW47|TKTC2_ARATH	Transketolase, chloroplastic	2530.3	17.2	GB	Basil	1
RY(+120.03)KAKEVHSLCGGK	Q9M4S8|TPIC_FRAAN	Triosephosphate isomerase, chloroplastic	1694.9	18.9	GB	Basil	1

[a] Peptides detected in given number of repetitions (N)