Supplemental Information

Linking Genomic and Metabolomic Natural Variation Uncovers Nematode Pheromone Biosynthesis

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Supplementary Information

Table of Contents

Supplementary Figures

Figure S1. GWAS and metabolomics of *P. pacificus* strains and mutants. Related to Figures 2 and 3.

Figure S2. MS/MS characterization of metabolites. Related to Figures 3 and 4.

Figure S3. Identification of phascr#3 in transgenic *C. elegans* expressing *hsp16.41*::*Ppa-uar-1* via co-injection with a synthetic sample and comparison of MS/MS spectra. Related to Figures 3 and 4.

Figure S4. Alignment of *Ppa-uar-1* amino acid sequence with best protein BLAST hits from human, mouse, *D. melanogaster*, and *E. coli*. Related to Figure 3.

Figure S5. Phylogeny of esterases in nematodes. Related to Figure 3.

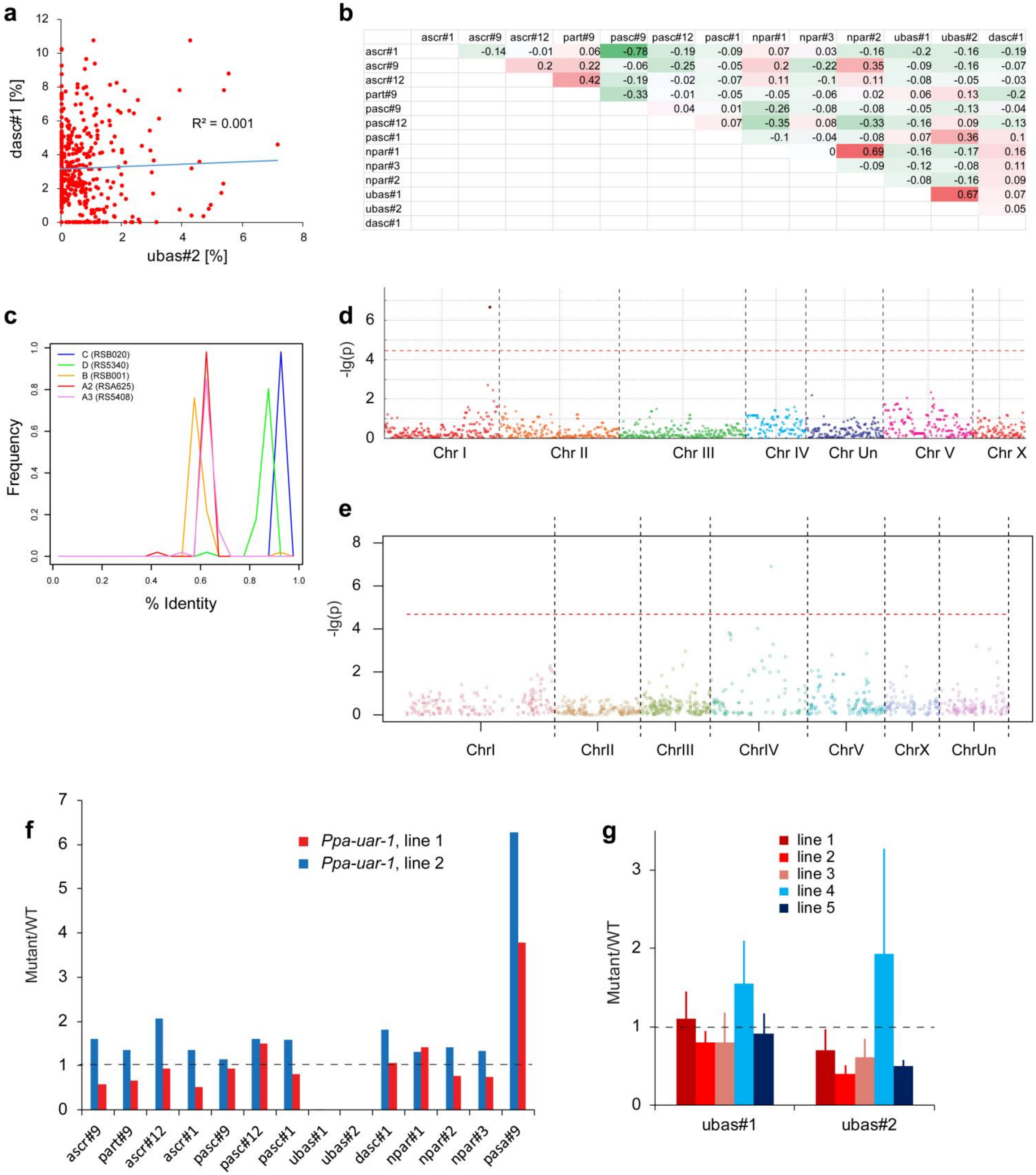
Supplementary Tables

Table S1. Amino acid sequence of *Ppa-uar-1* and Escherichia coli codon optimized *Ppa-uar-1*. Related to Figure 3.

Table S2. NMR spectroscopic data of ubas#6. Related to Figures 3 and 4.

Table S5. MS/MS data of new ubas ascarosides. Related to Figure 4.

Supplemental Figures



	ascr#1	ascr#9	ascr#12	part#9	pasc#9	pasc#12	pasc#1	npar#1	npar#3	npar#2	ubas#1	ubas#2	dasc#1
ascr#1		-0.14	-0.01	0.06	-0.78	-0.19	-0.09	0.07	0.03	-0.16	-0.2	-0.16	-0.19
ascr#9			0.2	0.22	-0.06	-0.25	-0.05	0.2	-0.22	0.35	-0.09	-0.16	-0.07
ascr#12				0.42	-0.19	-0.02	-0.07	0.11	-0.1	0.11	-0.08	-0.05	-0.03
part#9					-0.33	-0.01	-0.05	-0.05	-0.06	0.02	0.06	0.13	-0.2
pasc#9						0.04	0.01	-0.26	-0.08	-0.08	-0.05	-0.13	-0.04
pasc#12							0.07	-0.35	0.08	-0.33	-0.16	0.09	-0.13
pasc#1								-0.1	-0.04	-0.08	0.07	0.36	0.1
npar#1									0	0.69	-0.16	-0.17	0.16
npar#3										-0.09	-0.12	-0.08	0.11
npar#2											-0.08	-0.16	0.09
ubas#1												0.67	0.07
ubas#2													0.05
dasc#1													

Figure S1. GWAS and metabolomics of *P. pacificus* strains and mutants. Related to Figures 2 and 3. a) Correlation between dasc#1 and ubas#2. b) Pearson correlation coefficient matrix for all pairwise correlations among *P. pacificus* ascarosides. Cell color indicates negative (green) or positive (red) correlations; c) Clade assignment of collected *P. pacificus* strains. Collected *P. pacificus* strains were genotyped by RAD-seq and were compared with whole-genome-resequencing data of representative members for all la Reunion clades. The x-axis shows the pairwise percentage identity between a particular strain and each of the five clade representatives (Rödelsperger et al. 2014, McGaughran et al. 2016). Only sites that distinguish the five representative strains and that had sufficient coverage in all six strains (N≈20,000) were compared. The y-axis shows the frequency of strains at a given percentage identity value; d, e) Manhattan plots for ubas#2 and dasc#1, respectively. Results of genome wide association study (GWAS) using genomic data created with restriction site associated DNA (RAD) marker sequencing and metabolite abundances (ubas#2 in d) and dasc#1 in e)) as phenotypic dataset. Each dot represents the p-value for one SNP marker and its chromosomal location; f) Endo-metabolome ascaroside profile of *Ppa-uar-1* mutant strains. g) ubas#1 and ubas#2 levels in Contig39-snap124 mutant exo-metabolome. In f) and g) NDMM abundances are normalized to average levels in wildtype (RS2333, dashed line).

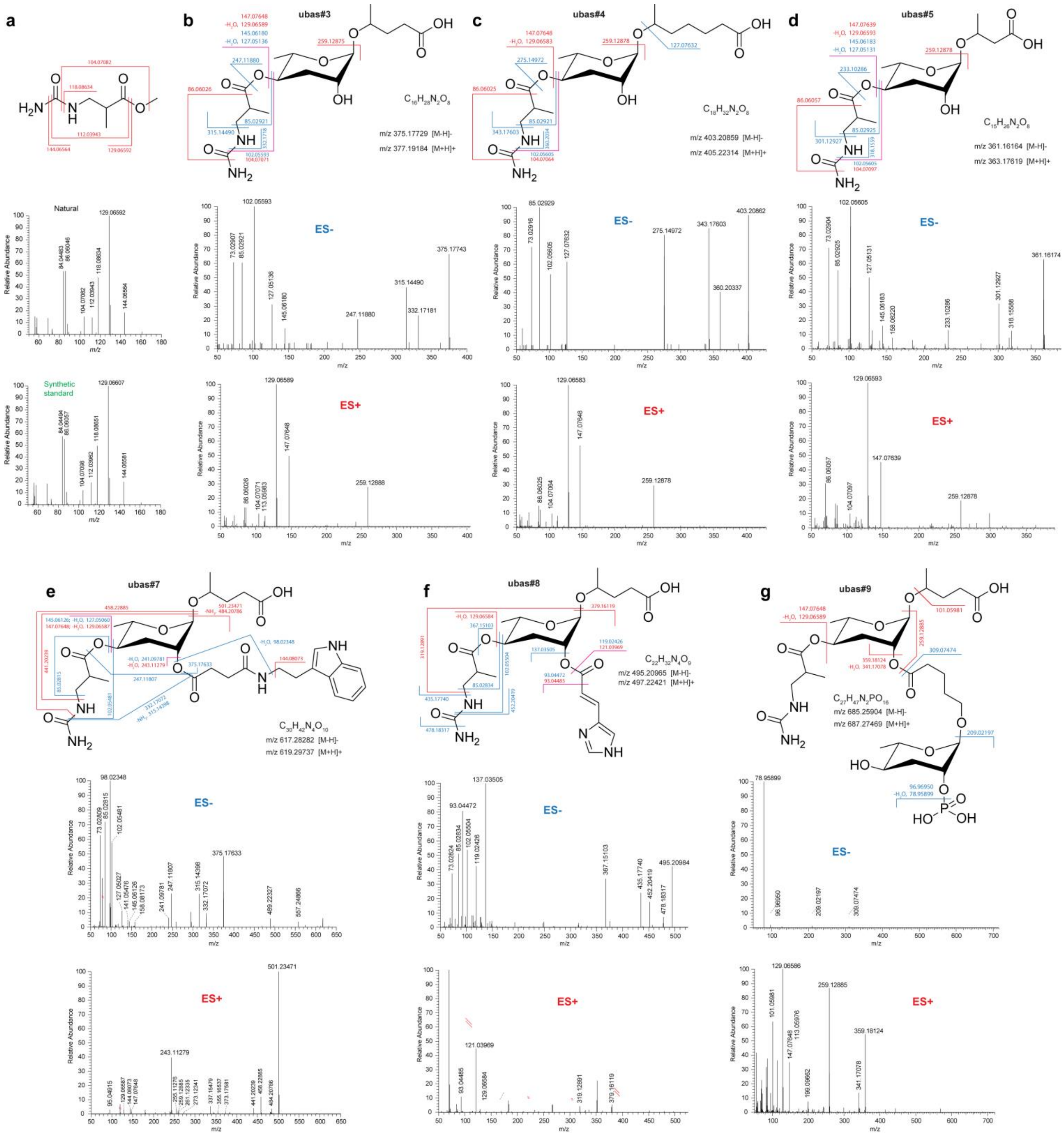


Figure S2. MS/MS characterization metabolites. Related to Figures 3 and 4. a) Structure of methyl ester of ureidoisobutyric acid showing characteristic ions observed in positive ionization mode MS/MS and fragmentation spectra for the methyl ester of natural and synthetic ureidoisobutyric acid; b) Fragmentation of ubas#3 in positive and negative ionization mode MS/MS. c) Fragmentation of ubas#4 in positive and negative ionization mode MS/MS. d)

Fragmentation of ubas#5 in positive and negative ionization mode MS/MS. e) Fragmentation of ubas#7 in positive and negative ionization mode MS/MS. f) Fragmentation of ubas#8 in positive and negative ionization mode MS/MS. g) Fragmentation of ubas#9 in positive and negative ionization mode MS/MS.

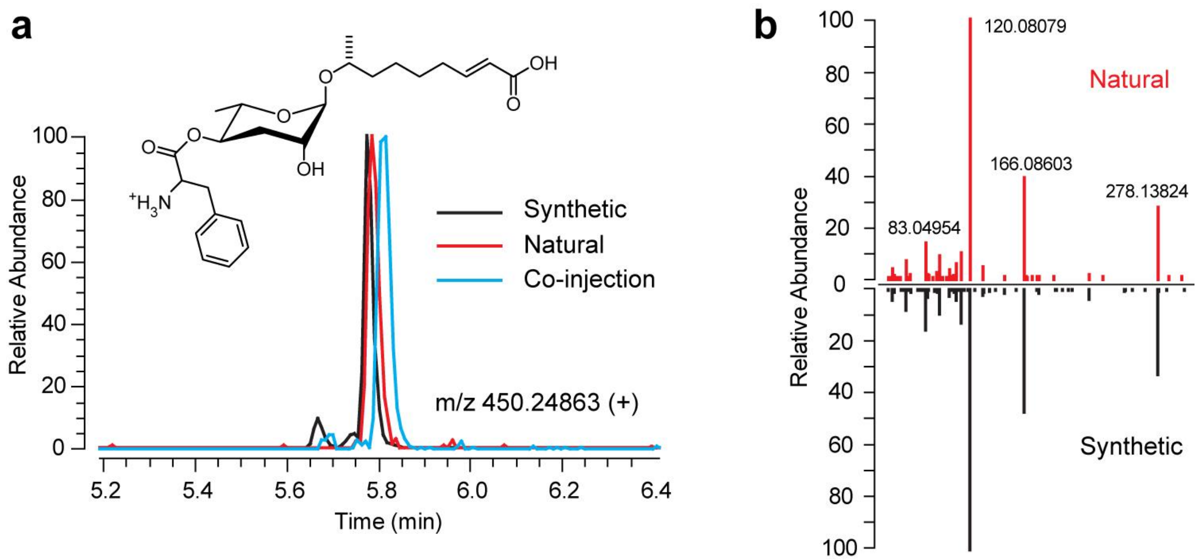


Figure S3. Identification of phascr#3 in transgenic *C. elegans* expressing *hsp16.41*::*Ppa-uar-1* via co-injection with a synthetic sample and comparison of MS/MS spectra. Related to Figures 3 and 4. a) Coinjection of metabolome sample from transgenic *C. elegans* expressing *hsp16.41::Ppa-uar-1* and synthetic phascr#3. b) Comparison of high-resolution MS/MS spectra of natural and synthetic phascr#3.

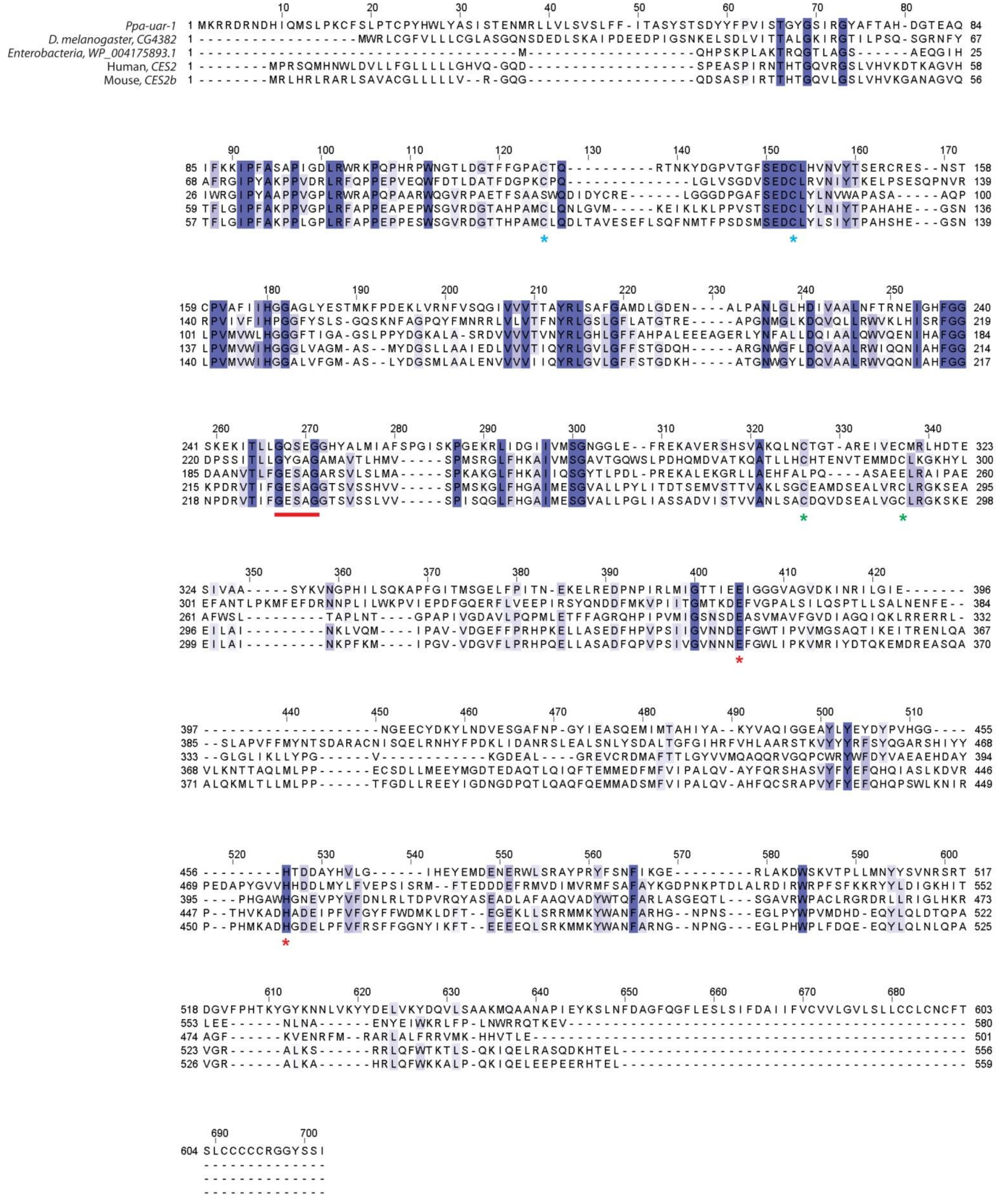


Figure S4. Alignment of *Ppa-uar-1* amino acid sequence with best protein BLAST hits from human, mouse, *D. melanogaster*, and *E. coli*. Related to Figure 3. Active site residues and serine hydrolase consensus sequence motif are marked with red asterisks and red line. Pairs of conserved cysteines forming disulfide bridges are marked with green and blue asterisks.

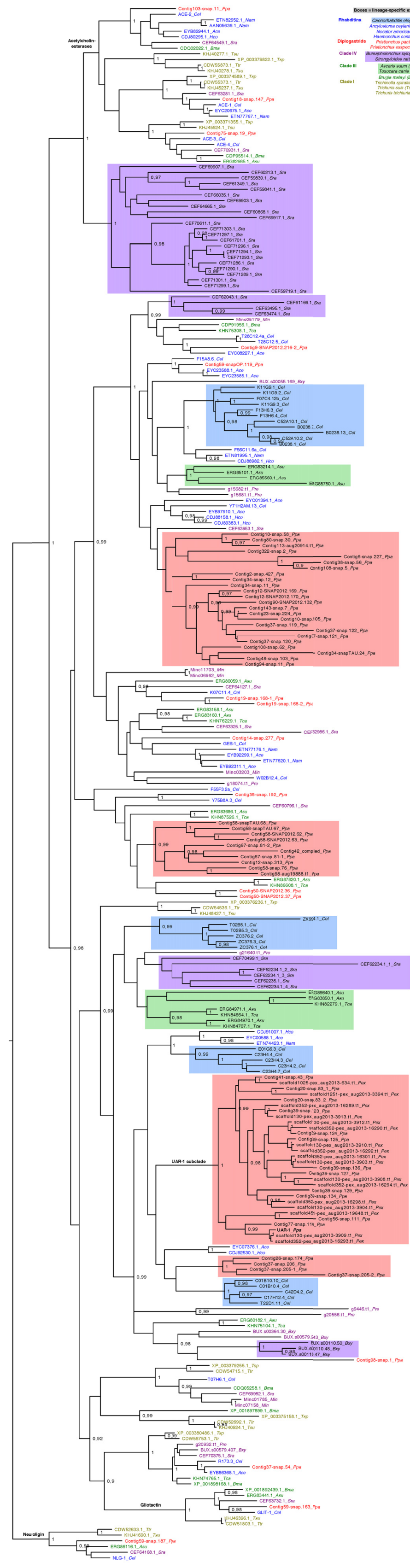


Figure S5. Phylogeny of esterases in nematodes. Related to Figure 3.

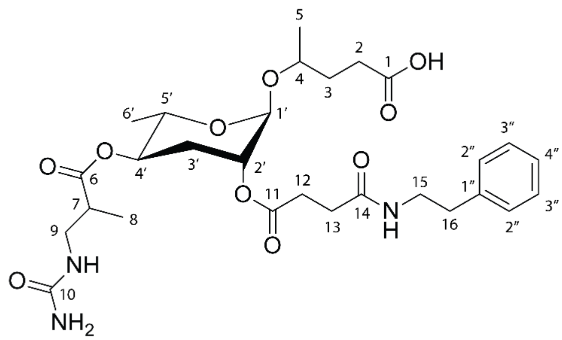
Supplemental Tables

Table S1. Amino acid sequence of *Ppa-uar-1* and *Escherichia coli* codon optimized *Ppa-uar-1*. Related to Figure 3.

Amino acid sequence of *Ppa-uar-1*
MKRRDRNDHIQMSLPKCFSLPTCPYHWLYASISTENMRLLVLSVSLFFITASYSTSDYYFPVISTGY
GSIRGYAFTAHDGTEAQIFKKIPFASAPIGDLRWRKPQPHRPWNGTLDGTFFGPACTQRTNKYDG
PVTGFSEDCLHVNVYTSERCRESNSTCPVAFIIHGGAGLYESTMKFPDEKLVRNFVSQGIVVVTTA
YRLSAFGAMDLGDENALPANLGLHDIVAALNFTRNEIGHFGGSKEKITLLGQSEGGHYALMIAFSP
GISKPGEKRLIDGIIVMSGNGGLEFREKAVERSHSVAKQLNCTGTAREIVECMRLHDTESIVAASYK
VNGPHILSQKAPFGITMSGELFPITNEKELREDPNPIRLMIGTTIEEIGGGVAGVDKINRILGIENGEE
CYDKYLNDVESGAFNPGYIEASQEMIMTAHIYAKYVAQIGGEAYLYEYDYPVHGGHTDDAYHVLGI
HEYEMDENERWLSRAYPRYFSNFIKGERLAKDWSKVTPLLMNYYSVNRSRTDGVFPHTKYGYKN
NLVKYYDELVKYDQVLSAAKMQAANAPIEYKSLNFDAGFQGFLESLSIFDAIIFVCVVLGVLSLLCCL
CNCFTSLCCCCCRGGYSSI

Escherichia coli* codon optimized *Ppa-uar-1
ATGAAACGTCGCGATCGCAATGACCATATTCAGATGAGCCTTCCGAAATGTTTCTCGTTGCCT
ACGTGTCCCTACCATTGGTTATACGCTTCAATTTCTACAGAGAATATGCGTTTATTGGTGTTAT
CCGTTTCCTTGTTCTTTATTACCGCCTCATACTCTACCTCTGATTACTACTTCCCAGTCATCTCG
ACTGGTTACGGCTCGATTCGCGGGTATGCATTTACCGCACACGACGGTACTGAAGCGCAAAT
TTTCAAAAAGATCCCCTTTGCCTCGGCACCCATCGGTGACTTGCGTTGGCGTAAACCCCAGCC
ACATCGTCCTTGGAACGGAACACTGGATGGTACTTTTTTCGGACCCGCTTGCACTCAGCGTAC
TAATAAGTACGACGGGCCCGTTACTGGGTTTTCGGAGGACTGTTTGCATGTGAATGTATACAC
ATCAGAGCGCTGCCGTGAGTCCAATTCTACTTGTCCTGTAGCCTTCATCATTCATGGAGGAGC
AGGTCTGTATGAGTCCACAATGAAATTTCCCGATGAAAAGCTGGTTCGTAATTTTGTGTCACAA
GGCATCGTCGTGGTAACGACTGCTTACCGCCTGAGCGCCTTTGGTGCTATGGACCTGGGAGA
TGAGAATGCATTACCGGCCAATCTTGGTCTTCACGATATTGTTGCAGCATTAAATTTTACTCGT
AACGAAATTGGCCATTTTGGGGGGTCGAAAGAAAAGATTACGCTTCTGGGGCAAAGCGAGGG
GGGTCATTATGCTCTGATGATCGCCTTTTCTCCAGGCATCTCAAAACCTGGTGAGAAACGTCT
GATTGATGGAATCATCGTAATGAGTGGAAACGGTGGACTTGAGTTCCGTGAAAAAGCCGTGG
AGCGCAGTCACAGTGTTGCTAAGCAATTAAATTGTACGGGAACGGCTCGTGAAATTGTGGAAT
GTATGCGTCTGCATGATACAGAAAGTATTGTCGCTGCCAGTTATAAAGTAAACGGTCCTCACA
TTTTGTCACAAAAGGCGCCCTTCGGGATTACAATGTCGGGTGAACTGTTTCCGATCACAAATG
AAAAAGAGTTGCGCGAAGATCCGAACCCTATTCGCTTAATGATCGGCACCACCATCGAAGAGA
TTGGCGGGGGTGTTGCAGGCGTAGATAAAATCAACCGTATCTTAGGGATTGAGAATGGAGAA
GAGTGTTACGACAAGTACTTAAACGATGTAGAATCAGGCGCTTTCAATCCTGGATACATCGAA
GCATCGCAAGAGATGATTATGACCGCTCATATTTACGCCAAGTACGTTGCCCAAATTGGGGGG
GAAGCCTACCTGTACGAGTATGATTATCCGGTACACGGCGGGCATACAGATGATGCCTACCA
CGTTTTGGGGATCCACGAATATGAAATGGATGAGAACGAACGCTGGCTTTCTCGCGCCTATCC
GCGTTATTTTTCCAACTTCATTAAAGGTGAACGTCTTGCTAAAGACTGGTCAAAGGTTACCCCA
TTACTGATGAATTACTACAGTGTGAACCGTTCCCGTACAGACGGTGTCTTCCCACACACCAAA
TATGGATACAAAAACAACCTGGTTAAATATTATGACGAATTAGTAAAGTATGATCAAGTCTTAA
GCGCCGCTAAAATGCAGGCCGCGAATGCGCCAATCGAGTACAAGAGTTTAAACTTTGATGCA
GGGTTCCAAGGGTTTCTGGAATCTCTGAGCATCTTCGACGCCATTATCTTTGTGTGTGTAGTG
TTGGGCGTCCTTTCCTTGTTATGCTGCCTGTGTAACTGTTTTACATCGCTGTGTTGCTGTTGCT
GTCGCGGGGGTTACTCATCAATCTAG

Table S2. NMR spectroscopic data of ubas#6. Related to Figures 3 and 4. Data were obtained via dqfCOSY spectra (solvent CD_3OD, resonance frequency 800 MHz)



Position	^{1}H [ppm]	^{1}H-^{1}H coupling constants (Hz)
1		
2-H_a 2-H_b	2.26 2.32	$J_{2a,2b}$ = 16, $J_{2a,3} \approx 7$ $J_{2b,3} \approx 7$
3	1.83	
4	3.83	$J_{4,5}$ = 6.2
5	1.15	
6		
7	2.68	$J_{7,8}$ = 7.3
8	1.13	
9	3.25	
10		
11		
12	2.65*	$J_{12,13}$ = 7.1
13	2.48*	
14		
15	3.40	$J_{15,16}$ = 7.5
16	2.79	
1′	4.77	$J_{1',2'}$ = 1.8
2′	4.81	$J_{2',3'eq}$ = 5.8, $J_{2',3'ax}$ = 6.1
3′-H_{ax} 3′-H_{eq}	2.02 2.09	$J_{3'eq,3'ax}$ = 13.5; $J_{3'eq,4'}$ = 4.2 $J_{3'ax,4'}$ = 11.4
4′	4.74	$J_{4',5'}$ = 9.1
5′	3.99	$J_{5',6'}$ = 6.2
6′	1.15	
1″		
2″	7.22	$J_{2'',3''}$ = 7.9
3″	7.28	$J_{3'',4''}$ = 7.7
4″	7.18	

*Signals could be interchanged

Table S5. MS/MS data of new ubas ascarosides. Related to Figure 4. Data for ubas#1 and #2 are included for comparison. The first entry for each compound (bold) is a molecular ion, the other are MS/MS fragments.

SMID	*RT*	*ES-*				*ES+*			
	(min)	*m/z (exp)*	*formula*	*m/z (calc)*	*Δ ppm*	*m/z (exp)*	*formula*	*m/z (calc)*	*Δ ppm*
ubas#1	5.88	**605.29340**	**$C_{27}H_{45}N_2O_{13}^-$**	**605.29271**	1.1	**607.30627**	**$C_{27}H_{47}N_2O_{13}^+$**	**607.30727**	-1.6
		73.02824	$C_3H_5O_2^-$	73.02950	-17.2	69.03397	$C_4H_5O^+$	69.03349	7.0
		85.02832	$C_4H_5O_2^-$	85.02950	-13.9	86.06026	$C_4H_8NO^+$	86.06004	2.6
		99.04409	$C_5H_7O_2^-$	99.04515	-10.7	95.04920	$C_6H_7O^+$	95.04914	0.6
		102.05503	$C_4H_8NO_2^-$	102.05605	-10.0	101.05979	$C_5H_9O_2^+$	101.05971	0.8
		127.05054	$C_5H_7N_2O_2^-$	127.05130	-6.0	113.05974	$C_6H_9O_2^+$	113.05971	0.3
		145.06137	$C_5H_9N_2O_3^-$	145.06187	-3.4	129.06584	$C_5H_9N_2O_2^+$	129.06585	-0.1
		247.11865	$C_{11}H_{19}O_6^-$	247.11871	-0.2	147.07642	$C_5H_{11}N_2O_3^+$	147.07642	0
		285.13428	$C_{14}H_{21}O_6^-$	285.13436	-0.3	199.09679	$C_{10}H_{15}O_4^+$	199.09649	1.5
		477.23398	$C_{22}H_{37}O_{11}^-$	477.23414	-0.3	242.10237	$C_{11}H_{16}NO_5^+$	242.10230	0.3
		545.26044	$C_{26}H_{41}O_{12}^-$	545.26035	0.2	259.12875	$C_{11}H_{19}N_2O_5^+$	259.12885	-0.4
		562.28735	$C_{26}H_{44}NO_{12}^-$	562.28690	-0.8	341.17017	$C_{16}H_{25}N_2O_6^+$	341.17071	-1.6
		588.26709	$C_{27}H_{42}NO_{13}^-$	588.26616	1.6	359.18100	$C_{16}H_{27}N_2O_7^+$	359.18128	-0.8
ubas#2	6.1	**619.30878**	**$C_{28}H_{47}N_2O_{13}^-$**	**619.30836**	0.7	**621.32208**	**$C_{28}H_{49}N_2O_{13}^-$**	**621.32292**	-1.4
		73.02822	$C_3H_5O_2^-$	73.02950	-17.5	86.06029	$C_4H_8NO^+$	86.06004	2.9
		85.02831	$C_4H_5O_2^-$	85.02950	-14.0	95.04923	$C_6H_7O^+$	95.04914	0.9
		99.04408	$C_5H_7O_2^-$	99.04515	-10.8	113.05981	$C_6H_9O_2^+$	113.05971	0.9
		102.05501	$C_4H_8NO_2^-$	102.05605	-10.2	115.07544	$C_6H_{11}O_2^+$	115.07536	0.7
		113.05989	$C_6H_9O_2^-$	113.06080	-8.0	129.06581	$C_5H_9N_2O_2^+$	129.06585	-0.3
		127.05053	$C_5H_7N_2O_2^-$	127.05130	-6.1	147.07651	$C_5H_{11}N_2O_3^+$	147.07642	0.6
		145.06133	$C_5H_9N_2O_3^-$	145.06187	-3.7	199.09660	$C_{10}H_{15}O_4^+$	199.09649	0.6
		261.13422	$C_{12}H_{21}O_6^-$	261.13436	-0.5	259.12875	$C_{11}H_{19}N_2O_5^+$	259.12885	-0.4
		299.14996	$C_{15}H_{23}O_6^-$	299.15001	-0.2	355.18661	$C_{17}H_{27}N_2O_6^+$	355.18636	0.7
		357.16727	$C_{16}H_{25}N_2O_7^-$	357.16672	1.5	373.19626	$C_{17}H_{29}N_2O_7^+$	373.19693	-1.8
		491.25000	$C_{23}H_{39}O_{11}^-$	491.24979	-0.4				
		559.27618	$C_{27}H_{43}O_{12}^-$	559.27600	0.3				
		576.30249	$C_{27}H_{46}NO_{12}^-$	576.30255	-0.1				
		602.28241	$C_{28}H_{44}NO_{13}^-$	602.28181	1.0				
ubas#3	4.58	**375.17731**	**$C_{16}H_{27}N_2O_8^-$**	**375.17729**	0.1	**377.19110**	**$C_{16}H_{29}N_2O_8^-$**	**377.19184**	-2.0
		73.02907	$C_3H_5O_2^-$	73.02950	-5.9	58.06572	$C_3H_8N^+$	58.06513	10.2
		85.02921	$C_4H_5O_2^-$	85.02950	-3.4	69.03393	$C_4H_5O^+$	69.03349	6.4
		102.05593	$C_4H_8NO_2^-$	102.05605	-1.2	86.06026	$C_4H_8NO^+$	86.06004	2.6
		127.05136	$C_5H_7N_2O_2^-$	127.05130	0.5	104.07066	$C_4H_{10}NO_2^+$	104.07060	0.6
		145.06180	$C_5H_9N_2O_3^-$	145.06187	-0.5	113.05983	$C_6H_9O_2^+$	113.05971	1.1
		247.11880	$C_{11}H_{19}O_6^-$	247.11871	0.4	129.06589	$C_5H_9N_2O_2^+$	129.06585	0.3
		315.14490	$C_{15}H_{23}O_7^-$	315.14493	-0.1	147.07648	$C_5H_{11}N_2O_3^+$	147.07642	0.4
		332.17181	$C_{15}H_{26}NO_7^-$	332.17148	1.0	259.12875	$C_{11}H_{19}N_2O_5^+$	259.12885	-0.4
ubas#4	5.32	**403.20853**	**$C_{18}H_{31}N_2O_8^-$**	**403.20859**	-0.1	**405.22241**	**$C_{18}H_{33}N_2O_8^+$**	**405.22314**	-1.8
		73.02916	$C_3H_5O_2^-$	73.02950	-4.7	58.06572	$C_3H_8N^+$	58.06513	10.2
		85.02929	$C_4H_5O_2^-$	85.02950	-2.5	69.03390	$C_4H_5O^+$	69.03349	5.9
		102.05605	$C_4H_8NO_2^-$	102.05605	0	86.06025	$C_4H_8NO^+$	86.06004	2.4
		127.07632	$C_7H_{11}O_2^-$	127.07645	-1.0	104.07064	$C_4H_{10}NO_2^+$	104.07060	0.4
		158.08220	$C_7H_{12}NO_3^-$	158.08227	-0.4	129.06583	$C_5H_9N_2O_2^+$	129.06585	-0.2
		275.14972	$C_{13}H_{23}O_6^-$	275.15001	-1.1	147.07648	$C_5H_{11}N_2O_3^+$	147.07642	0.4
		343.17603	$C_{17}H_{27}O_7^-$	343.17623	-0.6	259.12878	$C_{11}H_{19}N_2O_5^+$	259.12885	-0.3
		360.20337	$C_{17}H_{30}NO_7^-$	360.20278	1.6				

ubas#5	4.26	**361.16187**	$\mathbf{C_{15}H_{25}N_2O_8^-}$	**361.16164**	0.6	**363.17587**	$\mathbf{C_{15}H_{27}N_2O_8^+}$	**363.17619**	-0.9
		73.02904	$C_3H_5O_2^-$	73.02950	-6.3	129.06589	$C_5H_9N_2O_2^+$	129.06585	0.3
		85.02925	$C_4H_5O_2^-$	85.02950	-2.9	147.07635	$C_5H_{11}N_2O_3^+$	147.07642	-0.5
		102.05605	$C_4H_8NO_2^-$	102.05605	0	259.12863	$C_{11}H_{19}N_2O_5^+$	259.12885	-0.8
		127.05131	$C_5H_7N_2O_2^-$	127.05130	0.1				
		145.06183	$C_5H_9N_2O_3^-$	145.06187	-0.3				
		158.08220	$C_7H_{12}NO_3^-$	158.08227	-0.4				
		233.10286	$C_{10}H_{17}O_6^-$	233.10306	-0.9				
		301.12927	$C_{14}H_{21}O_7^-$	301.12928	0				
		318.15588	$C_{14}H_{24}NO_7^-$	318.15583	0.2				
ubas#6	6.71	**578.27173**	$\mathbf{C_{28}H_{40}N_3O_{10}^-}$	**578.27192**	-0.3	**580.28571**	$\mathbf{C_{28}H_{42}N_3O_{10}^+}$	**580.28647**	-1.3
		73.02829	$C_3H_5O_2^-$	73.02950	-16.6	105.06998	$C_8H_9^+$	105.06988	1.0
		85.02837	$C_4H_5O_2^-$	85.02950	-13.3	129.06587	$C_5H_9N_2O_2^+$	129.06585	0.2
		98.02375	$C_4H_4NO_2^-$	98.02475	-10.2	204.10205	$C_{12}H_{14}NO_2^+$	204.10191	0.7
		102.05508	$C_4H_8NO_2^-$	102.05605	-9.5	222.11258	$C_{12}H_{16}NO_3^+$	222.11247	0.5
		127.05060	$C_5H_7N_2O_2^-$	127.05130	-5.5	241.11823	$C_{11}H_{17}N_2O_4^+$	241.11828	-0.2
		145.06151	$C_5H_9N_2O_3^-$	145.06187	-2.5	402.19104	$C_{22}H_{28}NO_6^+$	402.19111	-0.2
		158.08199	$C_7H_{12}NO_3^-$	158.08227	-1.8	419.21796	$C_{22}H_{31}N_2O_6^+$	419.21766	0.7
		202.08754	$C_{12}H_{12}NO_2^-$	202.08735	0.9	462.22375	$C_{23}H_{32}N_3O_7^+$	462.22348	0.6
		247.11876	$C_{11}H_{19}O_6^-$	247.11871	0.2				
		315.14502	$C_{15}H_{23}O_7^-$	315.14493	0.3				
		332.17178	$C_{15}H_{26}NO_7^-$	332.17148	0.9				
		375.17755	$C_{16}H_{27}N_2O_8^-$	375.17729	0.7				
ubas#7	6.66	**617.28296**	$\mathbf{C_{30}H_{41}N_4O_{10}^-}$	**617.28282**	0.2	**619.29651**	$\mathbf{C_{30}H_{43}N_4O_{10}^+}$	**619.29737**	-1.4
		73.02809	$C_3H_5O_2^-$	73.02950	-19.3	95.04915	$C_6H_7O^+$	95.04914	0.1
		85.02815	$C_4H_5O_2^-$	85.02950	-15.9	129.06587	$C_5H_9N_2O_2^+$	129.06585	0.2
		98.02348	$C_4H_4NO_2^-$	98.02475	-13.0	144.08073	$C_{10}H_{10}N^+$	144.08078	-0.3
		102.05481	$C_4H_8NO_2^-$	102.05605	-12.1	147.07648	$C_5H_{11}N_2O_3^+$	147.07642	0.4
		127.05060	$C_5H_7N_2O_2^-$	127.05130	-5.5	243.11279	$C_{14}H_{15}N_2O_2^+$	243.11280	0
		141.05476	$C_7H_9O_3^-$	141.05572		255.11276	$C_{15}H_{15}N_2O_2^+$	255.11280	-0.2
		145.06126	$C_5H_9N_2O_3^-$	145.06187	-4.2	259.12885	$C_{11}H_{19}N_2O_5^+$	259.12885	0
		158.08173	$C_7H_{12}NO_3^-$	158.08227	-3.4	261.12335	$C_{14}H_{17}N_2O_3^+$	261.12337	-0.1
		241.09781	$C_{14}H_{13}N_2O_2^-$	241.09825		273.12341	$C_{15}H_{17}N_2O_3^+$	273.12337	0.1
		247.11807	$C_{11}H_{19}O_6^-$	247.11871	-2.6	337.15479	$C_{20}H_{21}N_2O_3^+$	337.15467	0.4
		315.14398	$C_{15}H_{23}O_7^-$	315.14493	-3.0	355.16537	$C_{20}H_{23}N_2O_4^+$	355.16523	0.4
		332.17072	$C_{15}H_{26}NO_7^-$	332.17148	-2.3	373.17581	$C_{20}H_{25}N_2O_5^+$	373.17580	0
		375.17633	$C_{16}H_{27}N_2O_8^-$	375.17729	-2.6	441.20239	$C_{24}H_{29}N_2O_6^+$	441.20201	0.9
		489.22327	$C_{25}H_{33}N_2O_8^-$	489.22424		458.22885	$C_{24}H_{32}N_3O_6^+$	458.22856	0.6
		557.24866	$C_{29}H_{37}N_2O_9^-$	557.25045		484.20786	$C_{25}H_{30}N_3O_7^+$	484.20783	0.1
						501.23471	$C_{25}H_{33}N_4O_7^+$	501.23438	0.7
ubas#8	4.8	**495.20953**	$\mathbf{C_{22}H_{31}N_4O_9^-}$	**495.20965**	-0.2	**497.22382**	$\mathbf{C_{22}H_{33}N_4O_9^+}$	**497.22421**	-0.8
		73.02824	$C_3H_5O_2^-$	73.02950	-17.3	66.03432	$C_4H_4N^+$	66.03383	7.4
		85.02834	$C_4H_5O_2^-$	85.02950	-13.6	93.04485	$C_5H_5N_2^+$	93.04472	1.4
		93.04472	$C_5H_5N_2^-$	93.04582	-11.8	121.03969	$C_6H_5N_2O^+$	121.03964	0.4
		102.05504	$C_4H_8NO_2^-$	102.05605	-9.9	129.06584	$C_5H_9N_2O_2^+$	129.06585	-0.1
		119.02426	$C_6H_3N_2O^-$	119.02509	-7.0	319.12891	$C_{16}H_{19}N_2O_5^+$	319.12885	0.2
		137.03505	$C_6H_5N_2O_2^-$	137.03565	-4.4	379.16119	$C_{17}H_{23}N_4O_6^+$	379.16121	-0.1
		367.15103	$C_{17}H_{23}N_2O_7^-$	367.15107	-0.1				
		435.17740	$C_{21}H_{27}N_2O_8^-$	435.17729	0.3				
		452.20419	$C_{21}H_{30}N_3O_8^-$	452.20384	0.8				
		478.18317	$C_{22}H_{28}N_3O_9^-$	478.18310	0.1				

ubas#9	5.1	**685.25964**	**$C_{27}H_{46}N_2PO_{16}^-$**	**685.25904**	0.9	**687.27307**	**$C_{27}H_{48}N_2PO_{16}^+$**	**687.27469**	-2.4
		78.95899	PO_3^-	78.95905	-0.8	101.05981	$C_5H_9O_2^+$	101.05971	1.0
		96.96950	$H_2PO_4^-$	96.96962	-1.2	113.05976	$C_6H_9O_2^+$	113.05971	0.4
		209.02197	$C_6H_{10}PO_6^-$	209.02205	-0.4	129.06586	$C_5H_9N_2O_2^+$	129.06585	0.1
		309.07474	$C_{11}H_{18}PO_8^-$	309.07448	0.8	147.07648	$C_5H_{11}N_2O_3^+$	147.07642	0.4
						199.09662	$C_{10}H_{15}O_4^+$	199.09649	0.7
						259.12885	$C_{11}H_{19}N_2O_5^+$	259.12885	0
						341.17078	$C_{16}H_{25}N_2O_6^+$	341.17071	0.2
						359.18124	$C_{16}H_{27}N_2O_7^+$	359.18128	-0.1