Supporting Information

Metabolomic "Dark Matter" Dependent on Peroxisomal β-Oxidation in *Caenorhabditis elegans*

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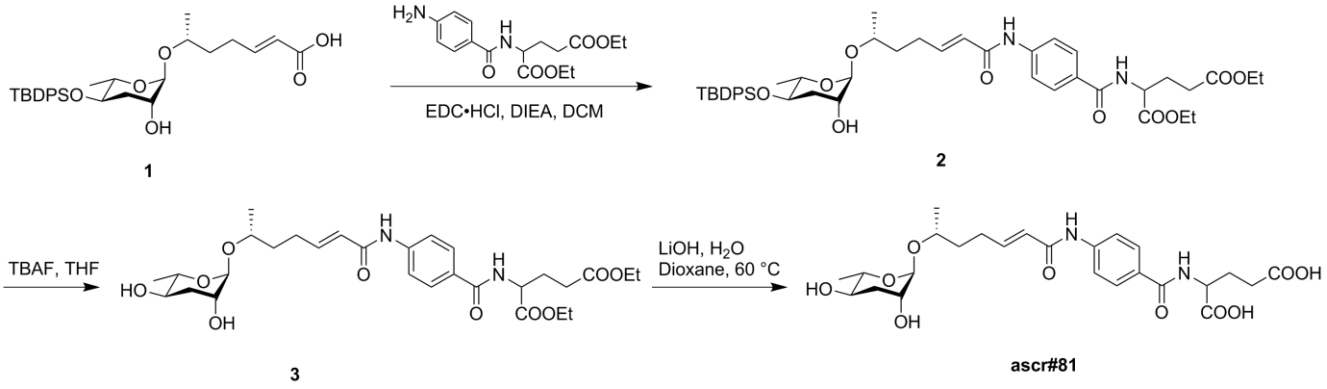
SUPPORTING METHODS

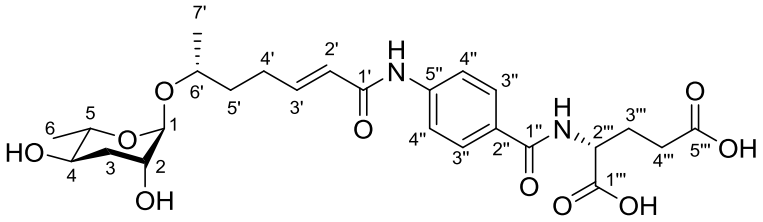
Synthesis of (4-((*R*,*E*)-6-(((2*R*,3*R*,5*R*,6*S*)-3,5-dihydroxy-6-methyltetrahydro-2*H*-pyran-2-yl)oxy)-hept-2-enamido)benzoyl)glutamic acid (ascr#81)



1 was prepared following a previously published procedure [1]. To a stirred solution of **1** (32 mg, 0.062 mmol) in dry dichloromethane (1 mL), *N*-(4-aminobenzoyl)-L-glutamic acid diethyl ester (72 mg, 0.223 mmol) and 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC•HCl) (46 mg, 0.240 mmol) were added at room temperature. The resulting mixture was stirred for 30 min, and *N*,*N*-diisopropylethylamine (42 μL, 0.241 mmol) was added. After 20 hours, the reaction was concentrated *in vacuo*. Flash column chromatography on silica using a gradient of 50-100% ethyl acetate in hexanes afforded **2** and some *N*-(4-aminobenzoyl)-L-glutamic acid diethyl ester (67.9 mg) as an off-white powder. The obtained mixture (10 mg) was dissolved in tetrahydrofuran (2 mL), and tetrabutylammonium fluoride solution (1 M in THF, 50 μL, 50 μmol) was added. After stirring overnight, the reaction was concentrated *in vacuo*. Flash column chromatography on silica using a gradient of 60-100% ethyl acetate in hexanes afforded **3** (3.1 mg, 5.3 μmol)**.**

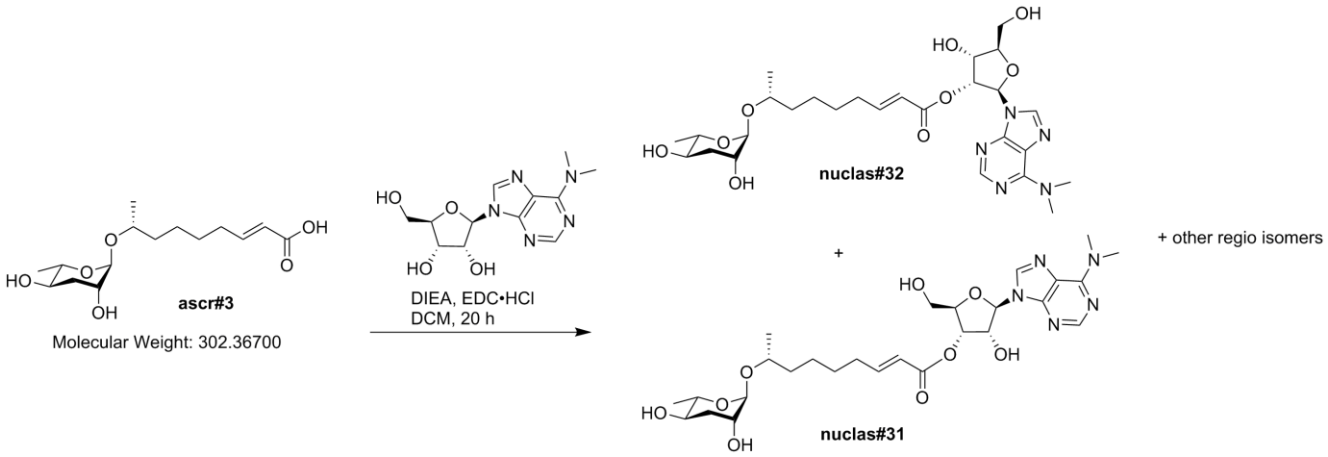
To a solution of **3** (3.1 mg, 5.3 μmol) in 1,4-dioxane (0.5 mL), lithium hydroxide monohydrate (1.4 mg, 0.032 mmol) in H_2O (0.2 mL) was added, and the resulting mixture was stirred at 60 °C for 12 hours. Glacial acetic acid (0.5 mL) was added, and the reaction was concentrated *in vacuo*. HPLC provided a pure sample of **ascr#81** (1.4 mg, 2.7 μmol 54%).

NMR Spectroscopic Data for ascr#81. ^{1}H (600 MHz), ^{13}C (151 MHz), HSQC and HMBC NMR spectroscopic data for **ascr#81** in methanol-d_4. Chemical shifts were referenced to ($CD_2\underline{H}OD$) = 3.31 ppm and ($\underline{C}D_2HOD$) = 49.00 ppm.



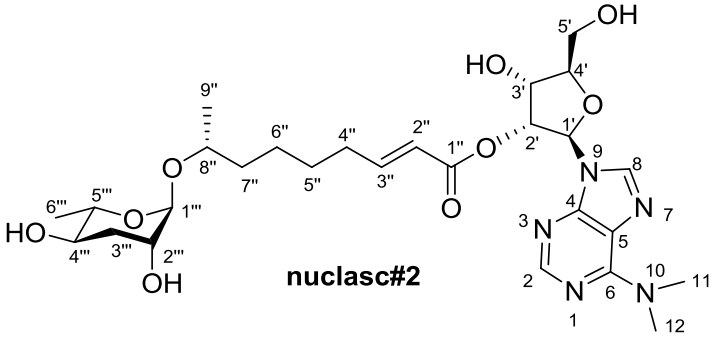
Position	δ ^{13}C [ppm]	δ ^{1}H [ppm]	^{1}H,^{1}H-coupling constants [Hz]	HMBC correlations
1	166.6			
2	125.0	6.16	$J_{2,3}$ = 15.3	C-1, C-3, C-4, C-5
3	147.3	6.99	$J_{3,4}$ = 6.9	C-1, C-2, C-4, C-5
4	29.2	2.39 (4a) 2.44 (4b)		C-2, C-3, C-5, C-6
5	36.7	1.72		C-3, C-4, C-6, C-7
6	71.4	3.86		C-1’, C-4, C-5
7	18.9	1.18	$J_{6,7}$ = 6.1	C-5, C-6
1’	97.1	4.68	$J_{1',2'} \approx$ 1.5	C-2’, C-3’, C-5’
2’	69.7	3.74	$J_{2',3'ax}$ = 3.1, $J_{2',3'eq}$ = 3.6,	C-1’, C-3’, C-4’
3’	35.8	1.79 (ax)	$J_{3'ax,4'}$ = 11.6, $J_{3'ax,3'eq}$ = 13.3	C-1’, C-2’, C-4’, C-5’
		1.97 (eq)	$J_{3'eq,4'}$ = 4.6	C-1’, C-2’, C-4’, C-5’, C-6’
4’	68.1	3.53	$J_{4',5'}$ = 9.3	C-2’, C-3’, C-5’, C-6’
5’	71.1	3.63	$J_{5',6'}$ = 6.1	C-1’, C-3’, C-4’, C-6’
6’	17.9	1.22		C-1’, C-4’, C-5’
1″	168.7			
2″	143.0			
3″	129.1	7.85	$J_{3'',4''}$ = 8.6	C-1″, C-2″, C-4″
4″	120.2	7.73		C-1″, C-2″, C-3″, C-5″
5″	130.6			
1‴	177.5			
2‴	54.9	4.50		C-1″, C-1‴, C-3‴, C-4‴
3‴	28.4	2.11 (3‴a) 2.28 (3‴b)		C-1‴, C-2‴, C-4‴
4‴	31.8	2.44		C-2‴, C-3‴, C-5‴
5‴	178.0			

Synthesis of (2*R*,3*R*,4*R*,5*R*)-2-(6-(dimethylamino)-9*H*-purin-9-yl)-4-hydroxy-5-(hydroxymethyl)-tetrahydrofuran-3-yl (*R*,*E*)-8-(((2*R*,3*R*,5*R*,6*S*)-3,5-dihydroxy-6-methyltetrahydro-2*H*-pyran-2-yl)oxy)non-2-enoate (nuclasc#2) and (2*R*,3*S*,4*R*,5*R*)-5-(6-(dimethylamino)-9*H*-purin-9-yl)-3-hydroxy-2-(hydroxymethyl)tetrahydrofuran-4-yl (*R*,*E*)-8-(((2*R*,3*R*,5*R*,6*S*)-3,5-dihydroxy-6-methyltetrahydro-2*H*-pyran-2-yl)oxy)non-2-enoate (nuclas#31)



To a stirred solution of **ascr#3** (42 mg, 0.139 mmol) in dry dichloromethane (1 mL), 1-(3-dimethyl-aminopropyl)-3-ethylcarbodiimide hydrochloride (EDC•HCl) (80 mg, 0.417 mmol) and 6-dimethyl-aminopurine-9-riboside (205 mg, 0.695 mmol) were added at room temperature. The resulting mixture was stirred for 30 min, and *N*,*N*-diisopropylethylamine (72.6 μL, 0.417 mmol) was added. After 20 hours, the reaction was concentrated *in vacuo*. Flash column chromatography on silica using a gradient of 0-20% methanol in dichloromethane afforded a crude mixture of aduasc#1 and byproducts (214 mg) as a clear oil. HPLC fractionation of a portion of this material provided a pure sample of **nuclas#32** (1.4 mg, 2.4μmol, 1.7%) and **nuclas#31** (3.1 mg, 5.3 μmol, 3.8%) whose HPLC retention times and MS/MS fragmentation patterns were identical to those of the natural products.

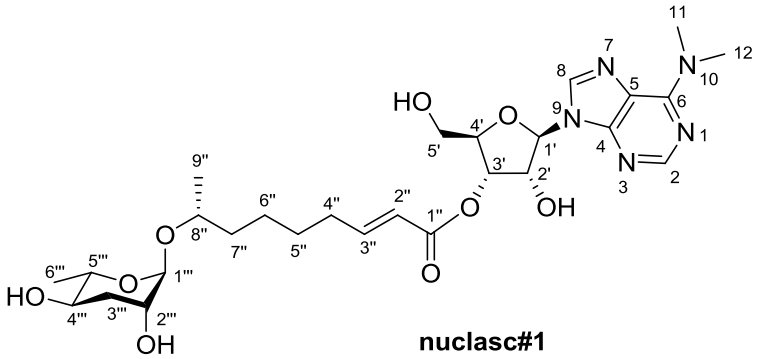
NMR Spectroscopic Data of nuclas#32. ^{1}H (600 MHz), HSQC, and HMBC NMR spectroscopic data were acquired in methanol-d_4. Chemical shifts were referenced to ($CD_2\underline{H}OD$) = 3.31 ppm and ($\underline{C}D_2HOD$) = 49.00 ppm.



Position	δ ^{13}C [ppm]	δ ^{1}H [ppm]	^{1}H,^{1}H-coupling constants [Hz]	HMBC correlations
1				
2	152.7			
3				
4	150.1			
5	121.4			
6	155.7			
7				
8	139.7			
9				
1′	88.3	6.22	$J_{1',2'}$ = 6.4	C-2′, C-4, C-8
2′	76.5	5.73	$J_{2',3'}$ = 5.3	C-1″
3′	71.1	4.63	$J_{3',4'}$ = 2.9	C-2′,
4′	88.3	4.20	$J_{4',5'}$ = 2.9,	
5′	63.2	3.91 (5′a) 3.77 (5′b)	$J_{4',5'}$ = 2.3, $J_{5',5'}$ = 12.4	
1″	166.3			
2″	120.7	5.90	$J_{2'',3''}$ = 15.8	C-1″
3″	152.2	7.03	$J_{3'',4''}$ = 7.1	C-1″
4″	33.1	2.24		C-2″, C-5″
5″, 6″	28.6, 26.3	1.37-1.58		
7″	37.9	1.59 (7″a) 1.53 (7″b)		
8″	72.3	3.77		
9″	19.2	1.11	$J_{8'',9''}$ = 6.2	C-7″, C-8″
1‴	97.4	4.63	$J_{1''',2'''} \approx$ 1.5	C-2‴, C-3‴, C-5‴
2‴	69.8	3.70	$J_{2''',3'''ax}$ = 3.0, $J_{2''',3'''eq}$ = 3.7	
3‴	35.8	1.74 (*ax*)	$J_{3'''ax,4'''}$ = 11.3, $J_{3'''ax,3'''eq}$ = 13.5	

		1.93 (*eq*)	, $J_{3'''eq,4'''}$ = 4.6	
4‴	68.1	3.51	$J_{4''',5'''}$ = 9.5	C-5‴
5‴	71.1	3.60	$J_{5''',6'''}$ = 6.3	
6‴	17.9	1.19		C-4‴, C-5‴

NMR Spectroscopic Data of nuclas#31. ^{1}H (600 MHz), HSQC, and HMBC NMR spectroscopic data were acquired in methanol-d_4. Chemical shifts were referenced to ($CD_2\underline{H}OD$) = 3.31 ppm and ($\underline{C}D_2HOD$) = 49.00 ppm.

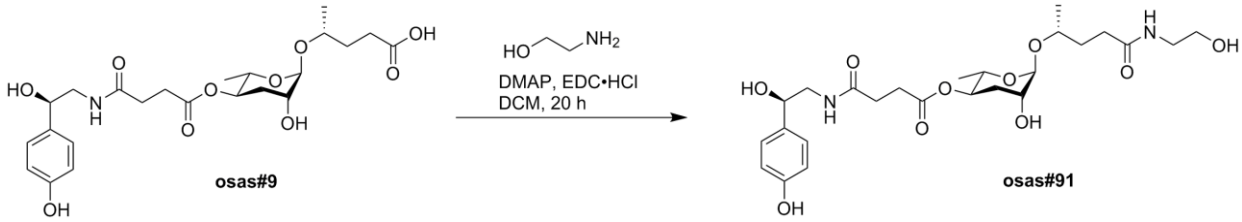


nuclasc#1

Position	δ ^{13}C [ppm]	δ ^{1}H [ppm]	^{1}H,^{1}H-coupling constants [Hz]	HMBC correlations
1				
2	152.7			
3				
4	150.1			
5	121.4			
6	155.7			
7				
8	140.1			
9				
1′	90.6	5.99	$J_{1',2'}$ = 7.4	C-2′, C-4, C-8
2′	73.6	5.01	$J_{2',3'}$ = 5.4	C-3′
3′	74.9	5.44	$J_{3',4'}$ = 1.7	C-1′, C-4′, C-5′, C-1″
4′	85.9	4.28		
5′	63.2	3.88 (5′a) 3.80 (5′b)	$J_{4',5'}$ = 2.3, $J_{4',5'}$ = 2.0, $J_{5',5'}$ = 12.5	
1″	166.8			
2″	121.7	6.00	$J_{2'',3''}$ = 15.5	C-1″, C-4″
3″	150.0	7.13	$J_{3'',4''}$ = 6.9	C-1″, C-4″, C-5″
4″	33.1	2.31		C-5″, C-6″
5″, 6″	28.8, 26.5	1.41-1.62		

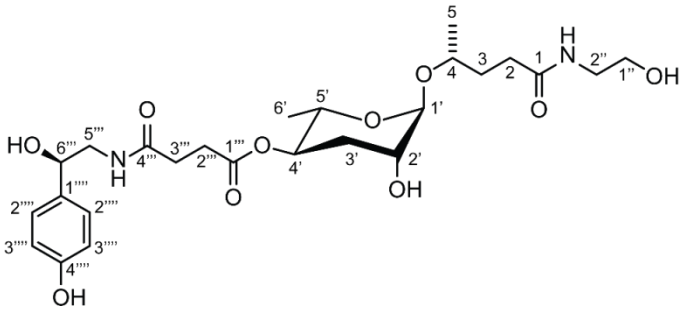
7″	37.9	1.58 (7″a) 1.52 (7″b)		
8″	72.3	3.80		
9″	19.2	1.13	$J_{8'',9''}$ = 6.1	C-7″, C-8″
1‴	97.4	4.65	$J_{1''',2'''} \approx$ 1.5	C-2‴, C-3‴, C-5‴, C-8″
2‴	69.8	3.72	$J_{2''',3'''ax}$ = 3.0, $J_{2''',3'''eq}$ = 3.8	C-4‴
3‴	35.8	1.77 (*ax*)	$J_{3'''ax,4'''}$ = 11.6, $J_{3'''ax,3'''eq}$ = 13.4	
		1.95 (*eq*)	$J_{3'''eq,4'''}$ = 4.5	
4‴	68.1	3.52	$J_{4''',5'''}$ = 9.5	C-5‴
5‴	71.1	3.63	$J_{5''',6'''}$ = 6.2	
6‴	18.0	1.22		C-4‴, C-5‴

(2*S*,3*R*,5*R*,6*R*)-5-hydroxy-6-(((*R*)-5-((2-hydroxyethyl)amino)-5-oxopentan-2-yl)oxy)-2-methyltetrahydro-2*H*-pyran-3-yl 4-(((*R*)-2-hydroxy-2-(4-hydroxyphenyl)ethyl)amino)-4-oxobutanoate (osas#91)



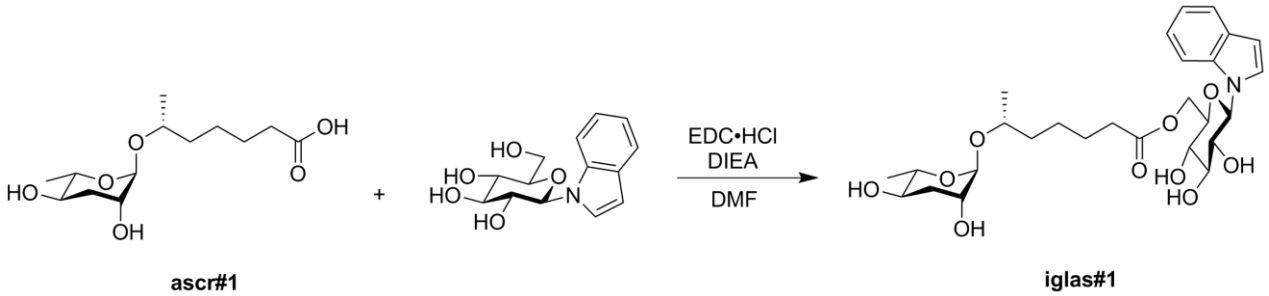
To a stirred solution of **osas#9** (2.6 mg, 5.4 μmol) in dry dichloromethane (0.4 mL), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC•HCl) (3.1 mg, 16 μmol) and ethanolamine (3.3 μL, 54 μmol) were added at room temperature. The resulting mixture was stirred for 30 min, and 4-dimethylaminopyridine (2.0 mg, 16 μmol) was added. After 20 hours, the reaction was concentrated *in vacuo*. Flash column chromatography on silica using a gradient of 0-20% methanol in dichloromethane afforded a mixture of aduasc#1 isomers together with reagent not separated from product (4 mg) as a clear oil. HPLC provided a pure sample of **osas#91** (0.1 mg, 0.19 μmol, 3.5%) identical to the natural product.

NMR Spectroscopic Data of osas#91. ^{1}H (800 MHz), HSQC, and HMBC NMR spectroscopic data were acquired in methanol-d_4. Chemical shifts were referenced to ($CD_2\underline{H}OD$) = 3.31 ppm and ($\underline{C}D_2HOD$) = 49.00 ppm.



Position	^{13}C [ppm]	^{1}H [ppm]	^{1}H-^{1}H coupling constants (Hz)	HMBC correlations
1″	61.3	3.59	$J_{1'',2''}$ = 6.0	C-2″
2″	42.7	3.29		C-1″
1	175.8	---		
2	33.0	2.30 (2a) 2.38 (2b)		C-1
3	33.8	1.82		
4	71.6	3.82		
5	18.7	1.16		C-3, C-4
1‴	174.2	---		
2‴	31.0	2.48	$J_{2''',3'''}$ = 6.6	C-1‴, C-3‴, C-4‴
3‴	30.3	2.58		C-1‴, C-2‴, C-4‴
4‴	173.1	---		
5‴	47.8	3.32 (5‴a) 3.39 (5‴b)	$J_{5'''a,5'''b}$ = 13.8, $J_{5'''a,6'''}$ = 8.2, $J_{5'''b,6'''}$ = 4.9	C-4‴, C-6‴
6‴	73.0	4.64		C-2⁗
1′	97.0	4.69	$J_{1',2'} \approx$ 1.5	C-4
2′	69.1	3.72	$J_{2',3'ax}$ = 3.0, $J_{2',3'eq}$ = 3.7	
3′	32.6	1.87 (ax) 2.04 (eq)	$J_{3'(ax),3'(eq)}$ = 12.9, $J_{3'(ax),4'}$ = 11.3, $J_{3'(eq),4'}$ = 5.3	
4′	71.3	4.87	$J_{4',5'}$ = 9.5	
5′	68.2	3.83	$J_{5',6'}$ = 6.2	
6′	17.8	1.15		C-4′, C-5′
1⁗	134.4	---		
2⁗	128.2	7.21	$J_{2'''',3''''}$ = 8.3	C-4⁗
3⁗	115.8	6.76		C-1⁗
4⁗	157.9	---		

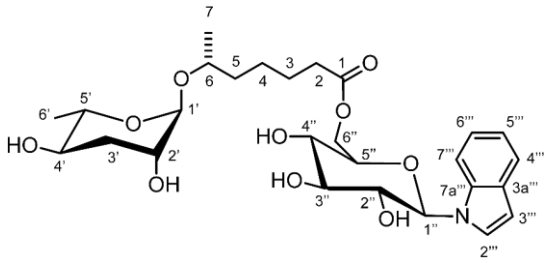
Synthesis of ((2*R*,3*S*,4*S*,5*R*,6*R*)-3,4,5-trihydroxy-6-(1*H*-indol-1-yl)tetrahydro-2*H*-pyran-2-yl)methyl (*R*)-6-(((2*R*,3*R*,5*R*,6*S*)-3,5-dihydroxy-6-methyltetrahydro-2*H*-pyran-2-yl)oxy)heptanoate (iglas#1)



ascr#1 **iglas#1**

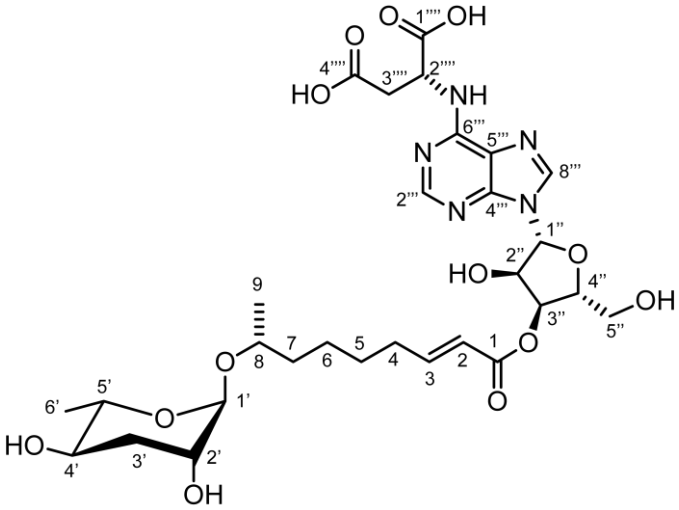
To a stirred solution of **ascr#1** (17 mg, 0.062 mmol) in dry dimethylformamide (0.5 mL), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDC•HCl) (39 mg, 0.203 mmol) and (3S,4S,5S,6R)-2-(Hydroxymethyl)-6-(1H-indol-1-yl)-tetrahydro-2H-pyran-3,4,5-triol (86 mg, 0.31 mmol) were added at room temperature. The resulting mixture was stirred for 30 min, and *N*,*N*-diisopropylethylamine (33 μL, 0.19 mmol) was added. After 20 hours, the reaction was concentrated *in vacuo*. Flash column chromatography on silica using a gradient of 0-20% methanol in dichloromethane afforded a crude mixture of **iglas#1** and byproducts as a clear oil. HPLC fractionation of a portion of this material provided a pure sample of **iglas#1** (5 μg) whose HPLC retention times and MS/MS fragmentation patterns were identical to those of the natural product.

NMR Spectroscopic Data of iglas#1. ^{1}H (800 MHz) NMR spectroscopic data were acquired in methanol-d_4. Chemical shifts were referenced to ($CD_2\underline{H}OD$) = 3.31 ppm and ($\underline{C}D_2HOD$) = 49.00 ppm.



Position	^{1}H [ppm]	^{1}H,^{1}H-coupling constants [Hz]
1	---	
2	2.34	
3	1.64	
4		
5		
6		
7		
1′	4.61	$J_{1',2'} \approx$ 1.5
2′	3.69	$J_{2',3'ax}$ = 3.0, $J_{2',3'eq}$ = 3.6
3′	1.75 (ax) 1.93 (eq)	$J_{3'(ax),3'(eq)}$ = 12.9, $J_{3'(ax),4'}$ = 11.3, $J_{3'(eq),4'}$ = 5.3
4′	3.50	$J_{4',5'}$ = 9.2
5′	3.59	$J_{5',6'}$ = 6.1
6′	1.20	
1″	5.45	$J_{1'',2''}$ = 9.0
2″	3.94	$J_{2'',3''}$ = 9.5
3″	3.60	$J_{3'',4''}$ = 9
4″	3.50	$J_{4'',5''}$ = 9
5″	3.79	$J_{5'',6''b}$ = 6.6
6″	4.43 (6″a) 4.24 (6″b)	$J_{6''a,6''b}$ = 12
2‴	7.36	$J_{2''',3'''}$ = 3.6
3‴	6.50	
4‴	7.53	$J_{4''',5'''}$ = 7.8; $J_{4''',6'''} \approx 2$
5‴	7.06	$J_{5''',6'''}$ = 7.5; $J_{5''',7'''} \approx 2$
6‴	7.15	$J_{6''',7'''}$ = 8.0
7‴	7.51	

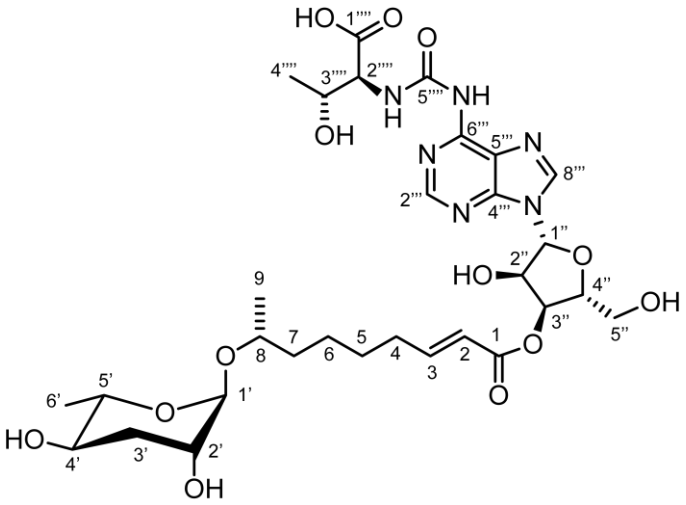
NMR Spectroscopic Data of nuclas#35. ^{1}H (800 MHz), HSQC, and HMBC NMR spectroscopic data were acquired in methanol-d_4. Chemical shifts were referenced to ($CD_2\underline{H}OD$) = 3.31 ppm and ($\underline{C}D_2HOD$) = 49.00 ppm. Absolute configuration of the aspartate moiety is proposed by analogy with the known tRNA nucleoside [2].



Position	^{13}C [ppm]	^{1}H [ppm]	^{1}H,^{1}H-coupling constants [Hz]	HMBC correlations
1	167.2	---		
2	121.5	5.99	$J_{2,3}$ = 15.9	C-1, C-4
3	151.8	7.13	$J_{3,4}$ = 7.0	C-1, C-4, C-5
4	33.0	2.30		C-2, C-3, C-5, C-6
5	28.8	1.54		
6	26.2	1.54 (6a) 1.44 (6b)		
7	37.8	1.59 (7a) 1.50 (7b)		
8	72.2	3.80	$J_{8,9}$ = 6.1	
9	19.1	1.13		C-7, C-8
1′	97.3	4.64		C-8, C-2′, C-3′, C-5′
2′	69.7	3.71	$J_{2',3'eq}$ = 2.9 $J_{2',3'ax}$ = 3.5	
3′	35.7	1.77 (ax) 1.95 (eq)	$J_{3'ax,3eq'}$ = 13.2 $J_{3'ax,4'}$ = 11.1 $J_{3'eq,4'}$ = 5.5	C-1′, C-2′, C-4′, C-5′
4′	68.0	3.52	$J_{4',5'}$ = 9.8	C-6′
5′	71.0	3.62	$J_{5',6'}$ = 6.2	
6′	17.9	1.21		C-4′, C-5′
1″	90.6	5.99	$J_{1'',2''}$ = 7.5	C-2″, C-4‴, C-8‴
2″	73.7	5.00	$J_{2'',3''}$ = 5.3	
3″	74.9	5.44	$J_{3'',4''}$ = 2.5	C-1, C-1″, C-5″
4″	86.0	4.28	$J_{4'',5''a}$ = 3.0 $J_{4'',5''b}$ = 3.0	C-3″

5″	63.1	3.88 (5″a) 3.79 (5″b)	$J_{5''a,5''b}$ = 13.1	C-3″, C-4″
2‴	153.3	8.25		
4‴	149.0	---		
5‴		---		
6‴		---		
8‴	141.1	8.24		C-4‴
1⁗, 4⁗	176.5, 177.2	---		
2⁗	52.6	4.98	$J_{2'''',3''''}$ = 6.2	
3⁗	39.7	2.94		C-1⁗, C-2⁗, C-4⁗

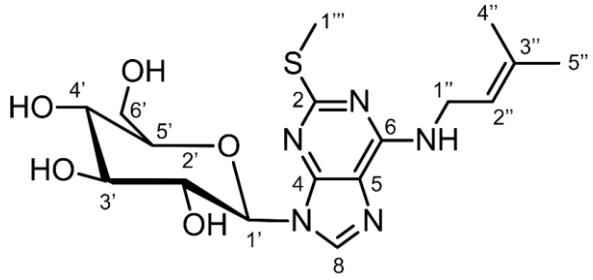
NMR Spectroscopic Data of nuclas#33. ^{1}H (800 MHz), HSQC, and HMBC NMR spectroscopic data were acquired in methanol-d_4. Chemical shifts were referenced to ($CD_2\underline{H}OD$) = 3.31 ppm and ($\underline{C}D_2HOD$) = 49.00 ppm. Absolute configuration of the threonine moiety is proposed by analogy with the known tRNA nucleoside t^6A [3].



Position	^{13}C [ppm]	^{1}H [ppm]	^{1}H,^{1}H-coupling constants [Hz]	HMBC correlations
1	167.1	---		
2	121.5	6.01	$J_{2,3}$ = 15.7	C-1, C-4
3	151.9	7.13	$J_{3.4}$ = 6.8	C-1, C-4, C-5
4	33.0	2.31		C-2, C-3, C-5, C-6
5	28.8	1.54		C-4, C-6, C-7
6	26.2	1.54 (6a) 1.45 (6b)		
7	37.9	1.58 (7a) 1.50 (7b)		

8	72.1	3.79	$J_{8,9}$ = 6.2	C-6, C-7, C-1′
9	19.0	1.13		C-7, C-8
1′	97.3	4.64		C-8, C-2′, C-3′, C-5′
2′	69.7	3.72	$J_{2',3'eq}$ = 2.9 $J_{2',3'ax}$ = 3.1	C-4′
3′	35.7	1.77 (ax) 1.94 (eq)	$J_{3'ax,3eq'}$ = 13.2 $J_{3'ax,4'}$ = 11.2 $J_{3'eq,4'}$ = 5.2	C-1′, C-2′, C-4′, C-5′
4′	68.0	3.52	$J_{4',5'}$ = 9.5	C-5′, C-6′
5′	71.0	3.62	$J_{5',6'}$ = 6.2	C-3′, C-4′
6′	17.9	1.21		C-4′, C-5′
1″	90.3	6.10	$J_{1'',2''}$ = 7.0	C-2″, C-4‴, C-8‴
2″	74.0	5.03	$J_{2'',3''}$ = 5.3	C-1″
3″	74.5	5.45	$J_{3'',4''}$ = 2.7	C-1, C-1″
4″	85.8	4.30	$J_{4'',5''a}$ = 3.0 $J_{4'',5''b}$ = 3.0	
5″	62.4	3.89 (5″a) 3.82 (5″b)	$J_{5''a,5''b}$ = 12.8	C-3″, C-4″
2‴	152.1	8.62		C-4‴, C-6‴
4‴	151.1	---		
5‴	121.8	---		
6‴	151.8	---		
8‴	143.3	8.51		C-4‴, C-5‴
1⁗	176.6	---		
2⁗	61.3	4.37	$J_{2'''',3''''}$ = 3.5	C-1⁗, C-3⁗, C-4⁗ C-5⁗
3⁗	68.9	4.34	$J_{3'''',4''''}$ = 6.5	
4⁗	20.0	1.25		C-2⁗, C-3⁗
5⁗	155.7	---		

NMR Spectroscopic Data of pugl#1. ^{1}H (800 MHz), HSQC, and HMBC NMR spectroscopic data were acquired in methanol-d_4. Chemical shifts were referenced to ($CD_2\underline{H}OD$) = 3.31 ppm and ($\underline{C}D_2HOD$) = 49.00 ppm.



Position	^{13}C [ppm]	^{1}H [ppm]	^{1}H,^{1}H-coupling constants [Hz]	HMBC correlations
2	167.2	---		
4	151.0	---		
5	117.4	---		
6	154.7	---		
8	139.3	8.10	$J_{8,1'} \approx 1$	C-4, C-5, C-6, C-8, C-1′
1′	84.4	5.50	$J_{1',2'} = 9.0$	C-4, C-8, C-2′, C-3′, C-5′
2′	73.0	4.09	$J_{2',3'} = 9.6$	C-1′, C-3′, C-4,
3′	78.6	3.55		C-2′, C-4′, C-5′
4′	70.8	3.52	$J_{4',5'} = 10.0$	C-3′, C-5′, C-6′
5′	80.8	3.56	$J_{5',6'a} = 6.0$ $J_{5',6'b} = 3.0$	C-1′, C-3′, C-4′, C-6′
6′	62.2	3.72 (6′a) 3.87 (6′b)	$J_{6'a,6'b} = 13.4$	C-1′, C-4′, C-5′
1″	39.1	4.17	$J_{1'',2''} = 7.0$ $J_{1'',4''} \approx 2$ $J_{1'',5''} \approx 2$	
2″	121.7	5.37	$J_{2'',4''} \approx 2$ $J_{2'',5''} \approx 2$	C-1″, C-4″, C-5″
3″	136.5	---		
4″	17.9	1.77		C-1″, C-2″, C-3″, C-5″
5″	25.7	1.76		C-4″
1‴	14.3	2.56		C-2

SUPPORTING FIGURES

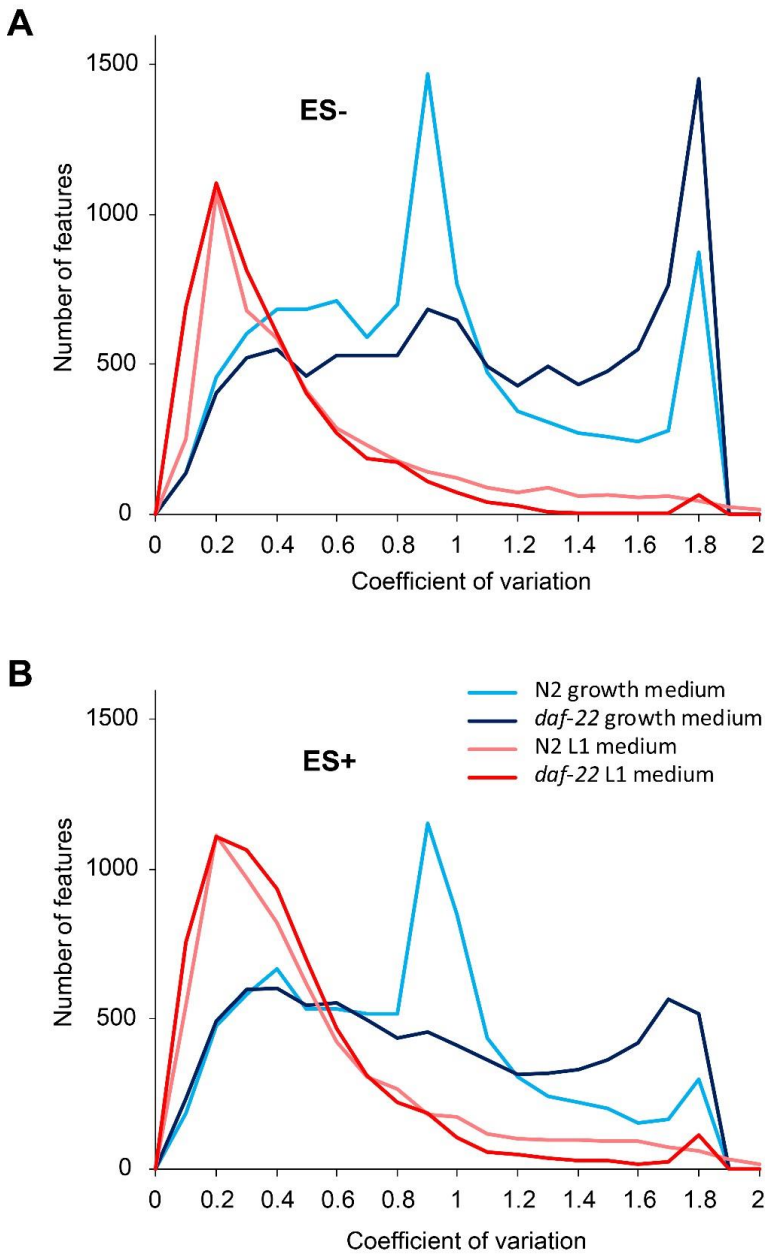


Figure S1. *C. elegans* growth medium is more variable than L1 medium. Coefficients of variation (CV) for peak areas were computed for all detected features in negative (A) and positive (B) ionization modes across replicates. Here we plot distributions of CV across all features for N2 and *daf-22* samples, number of bins equals 20. Growth medium samples (blue lines) have higher number of features with larger CV.

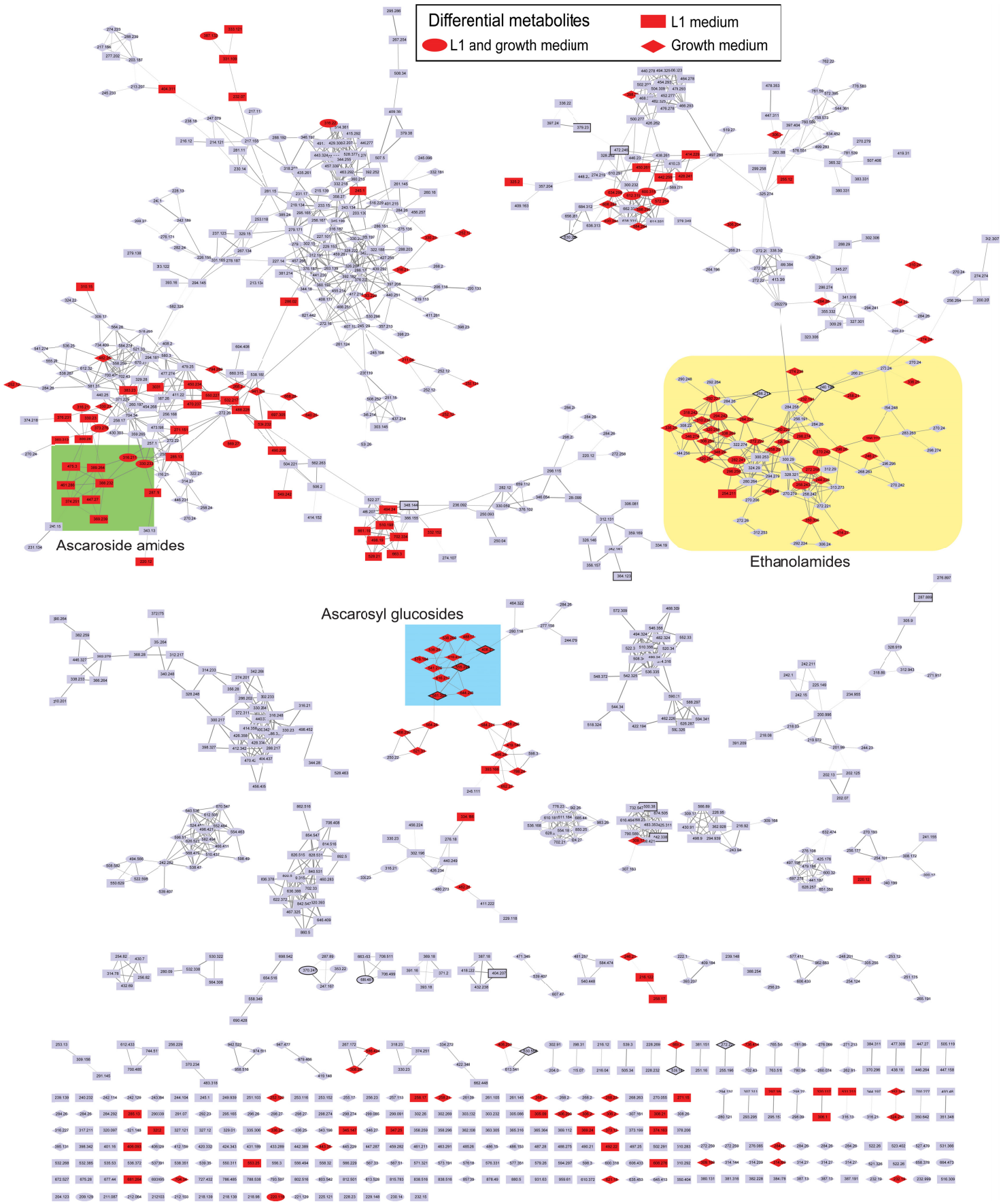


Figure S2. Molecular network of *C. elegans daf-22*-dependent features, positive ionization mode. Nodes representing redundant features are marked with black frames. For MS/MS data of *daf-22* dependent features, please refer to Tables S2-S17.

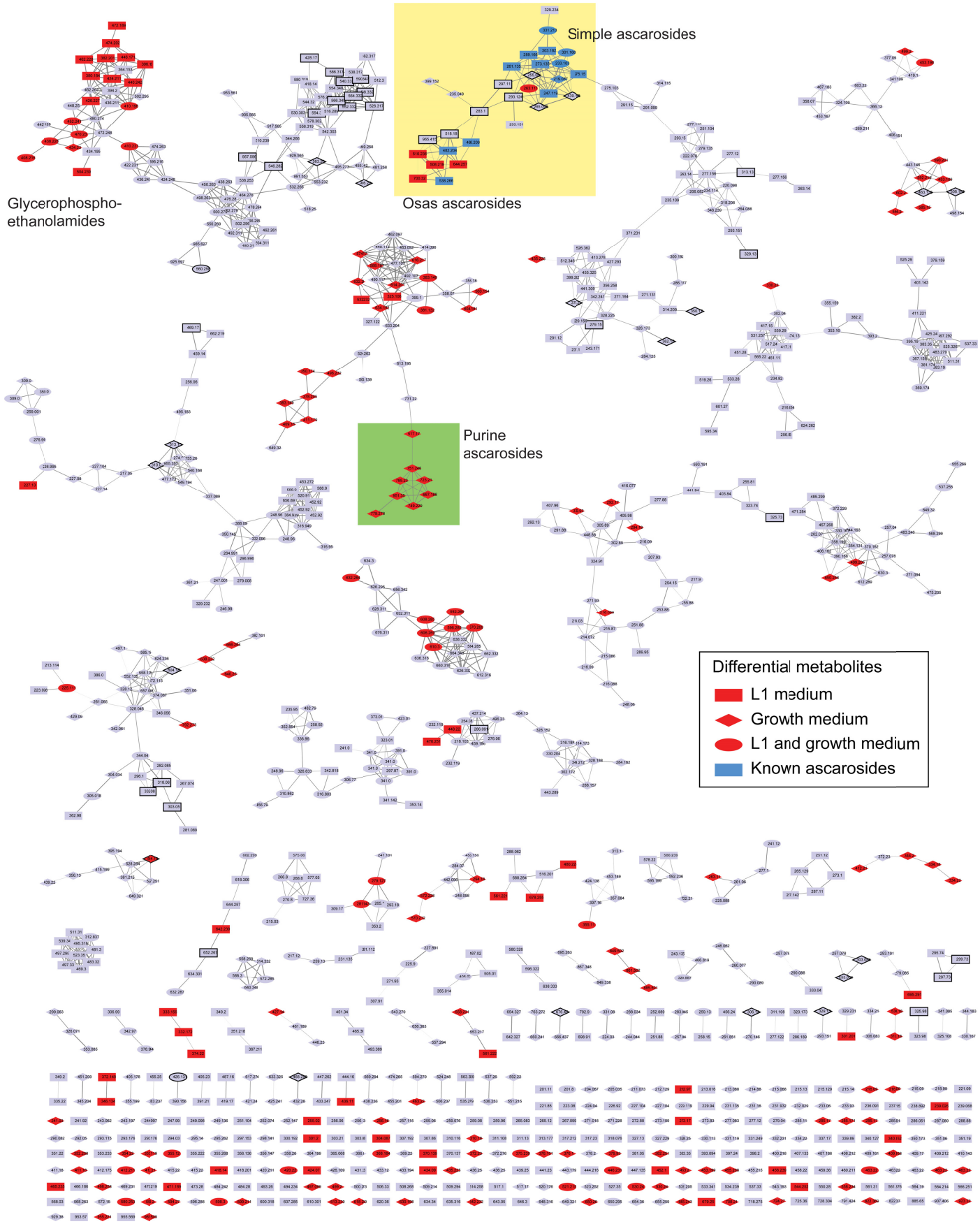


Figure S3. Molecular network of *C. elegans daf-22*-dependent features, negative ionization mode. Nodes representing redundant features are marked with black frames. For MS/MS data of *daf-22* dependent features, please refer to Tables S2-S17.

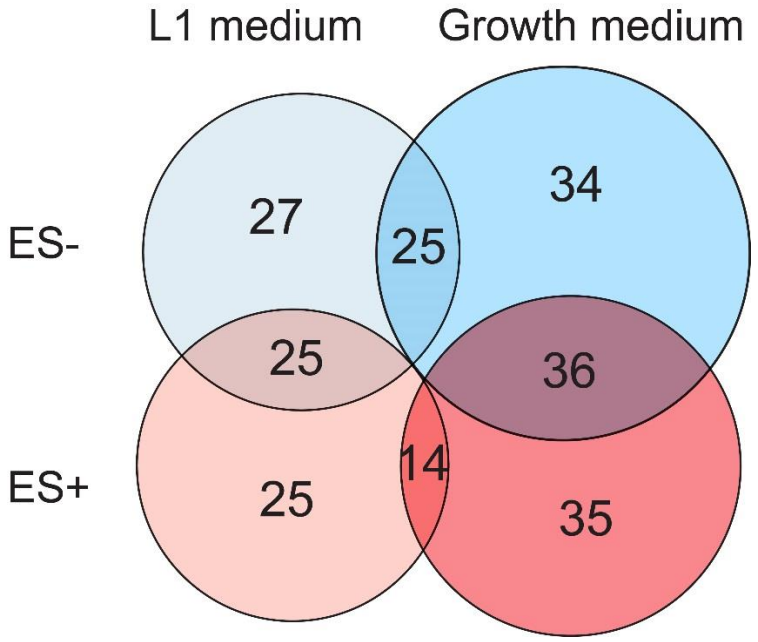


Figure S4. Venn diagram highlighting developmental stage specificity of *C. elegans daf-22* dependent metabolites.

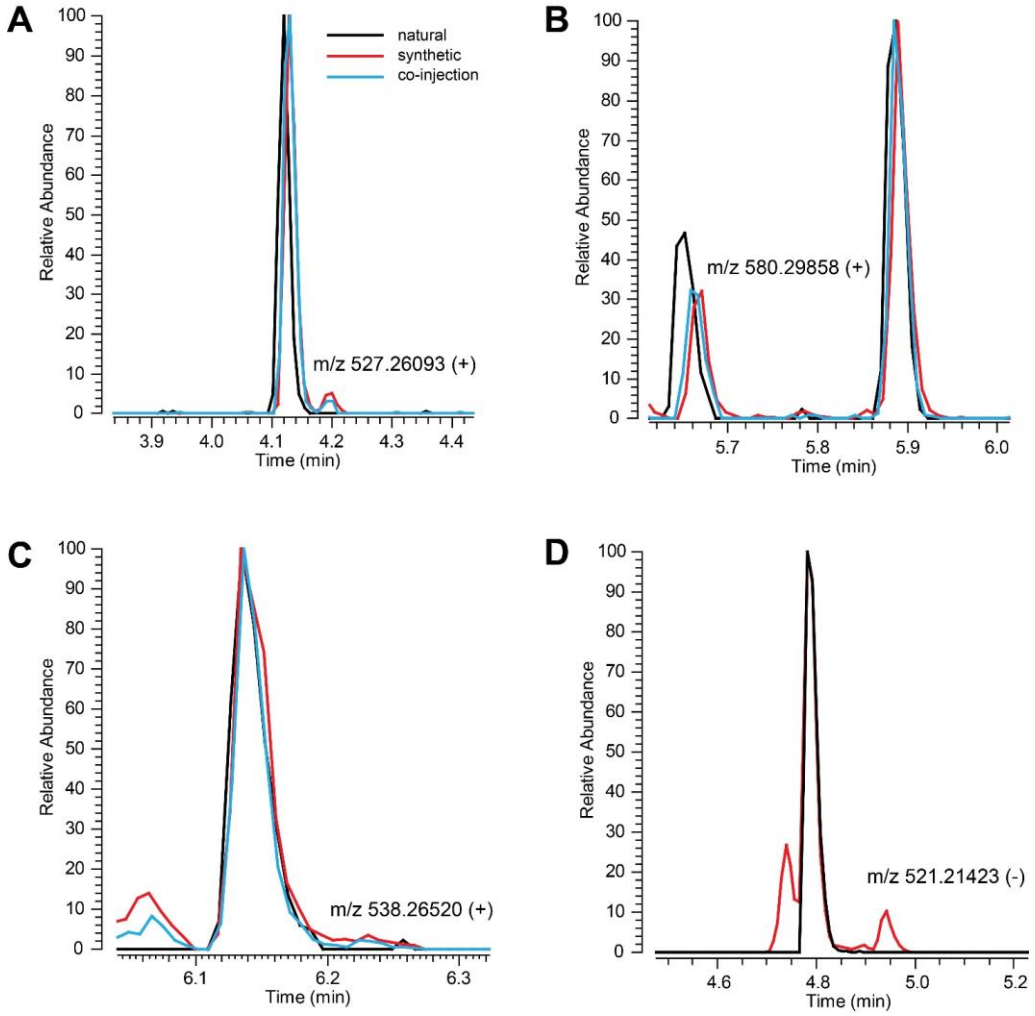


Figure S5. EICs of co-injection experiments of synthetic compounds with natural samples. (A) osas#91, (B) nuclas#3, (C) iglas#1, (D) ascr#81.

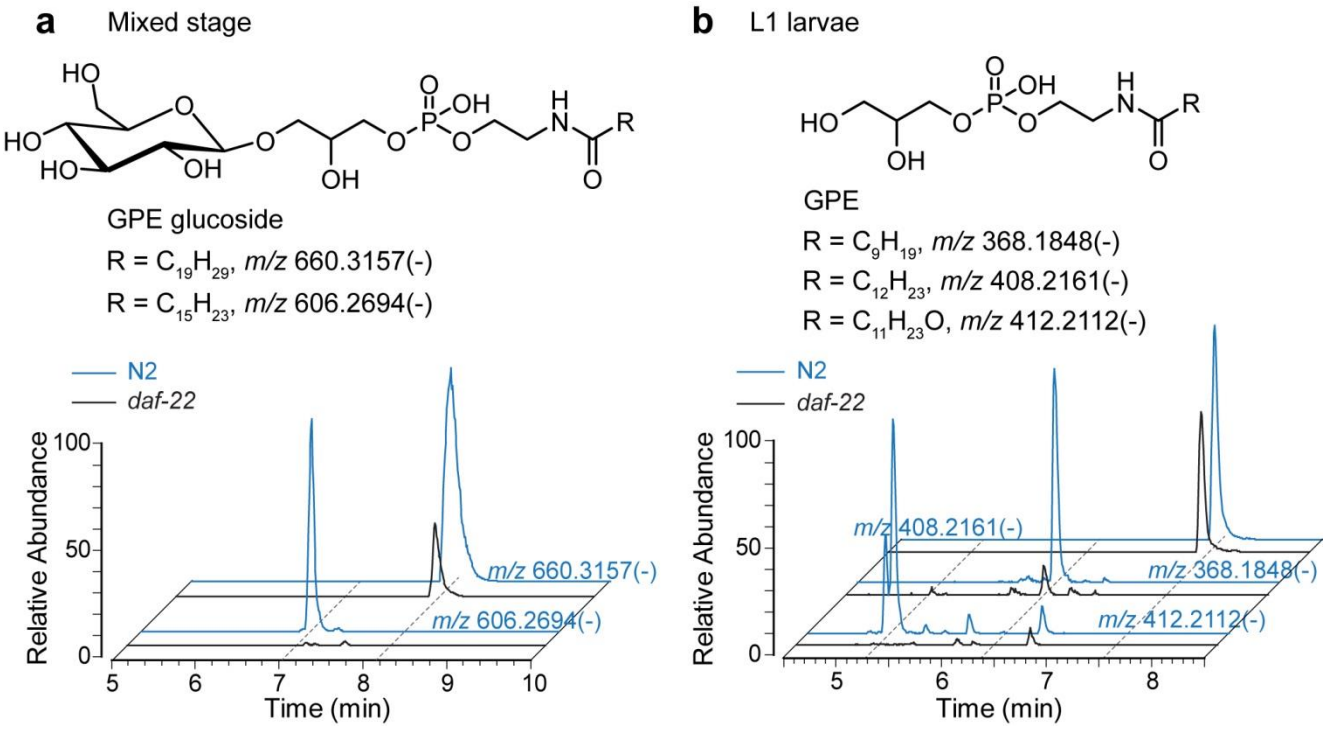


Figure S6. a) Levels of different GPE glucosides in growth medium are differently affected by *daf-22* mutation. b) *daf-22* has different effects on various GPEs in L1 medium. The double peak with m/z 412.2112 at 5.3 min is undetectable in *daf-22*, m/z 368.1848 at 6.4 min is significantly reduced compared to wildtype but still present in *daf-22*, m/z 408.2161 at 7.5 min is unchanged in *daf-22*.

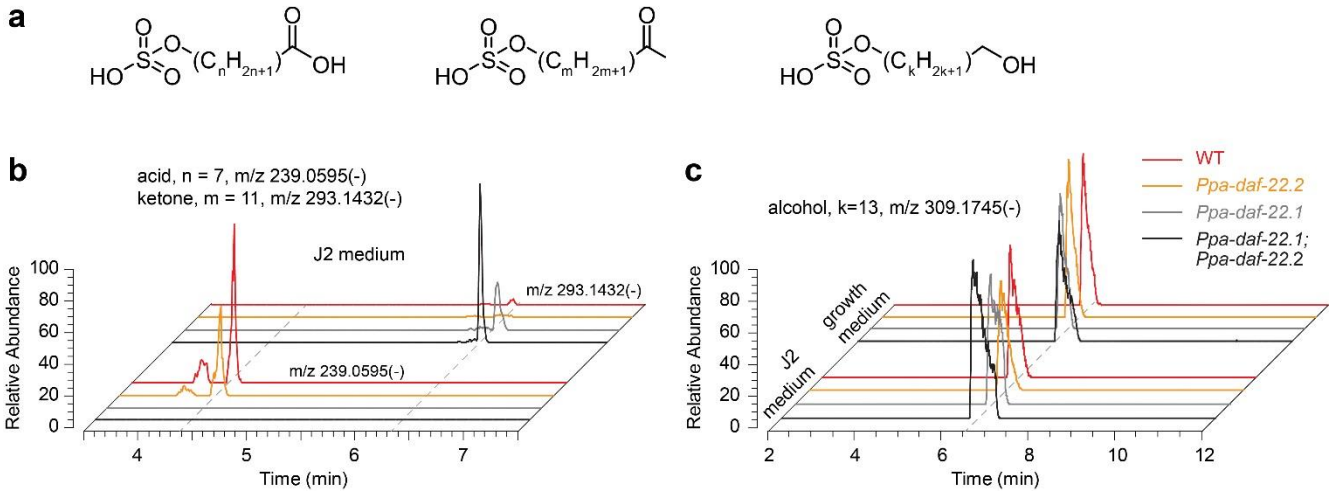


Figure S7. a) Generic structures of *daf-22* dependent sulfates in *P. pacificus.* b) EICs (ES-) of two sulfates from *P. pacificus* J2 medium. A medium chain acid (m/z 239.0595) is present in wildtype and *Ppa-daf-22.2* but absent in *Ppa-daf-22.1* and the double mutant. A longer chain putative methylketone (m/z 293.1432) accumulates in the double mutant and *Ppa-daf-22.1*. c) Production of some sulfates is not dependent on *Ppa-daf-22*.

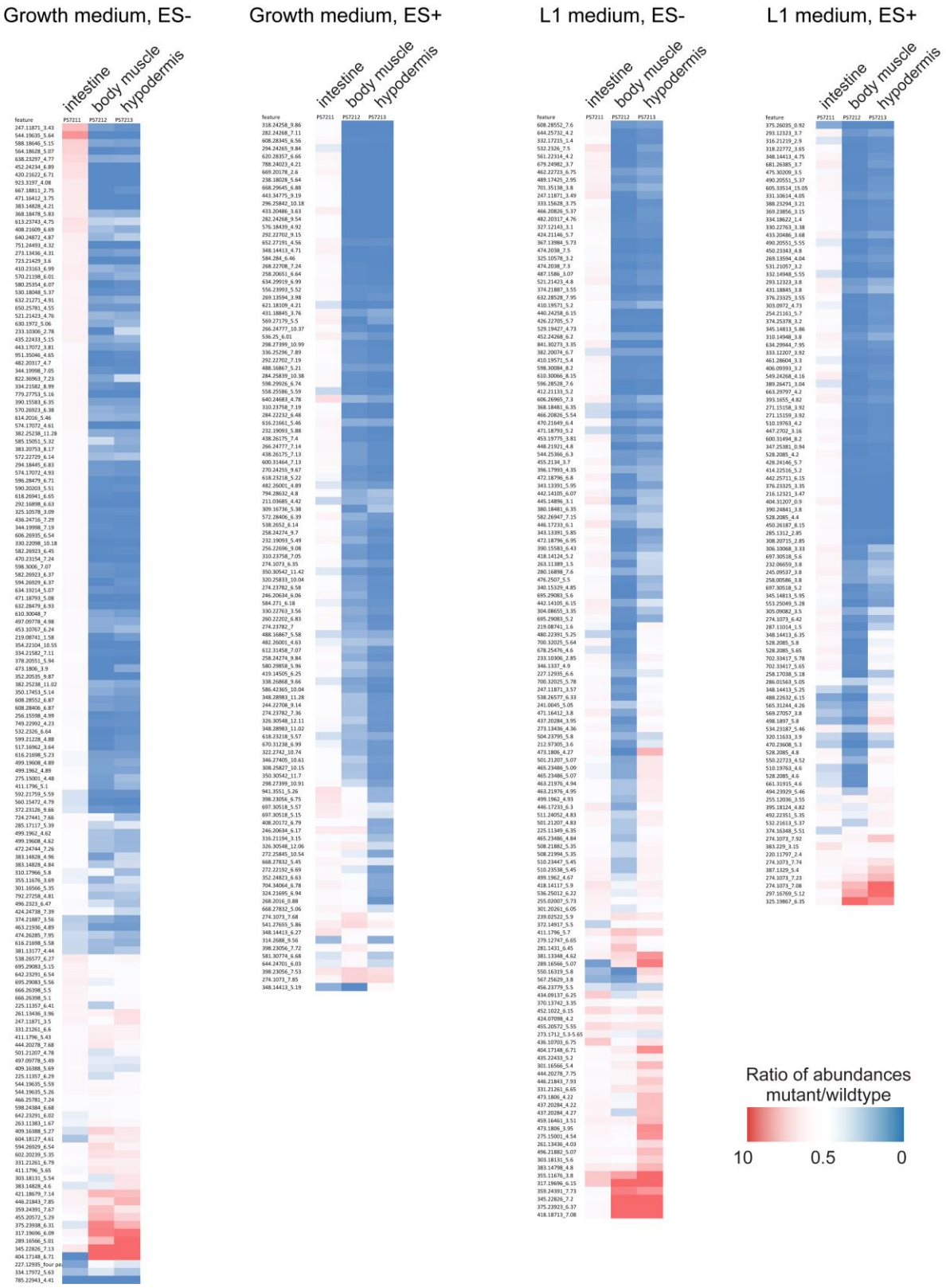


Figure S8. Tissue specific *daf-22* rescue in *C. elegans.* Heat maps showing expression of *daf-22*-dependent metabolites in tissue specific rescue lines relative to N2 levels in growth medium and L1 metabolomes.

SUPPORTING TABLES

Table S1. Comparison of feature extraction methods for the *C. elegans* data set. The data set consisted of 6 MS data files obtained for growth medium samples (3 independent replicates each for wildtype (N2) and *daf-22*), run in the negative ionization mode.

	XCMS profile	XCMS centroid	MS-DIAL
Total number of features.	10,350	114,675	33,956
Number of differential features (down in *daf-22*).	759	3,465	1,676
Number of verified differential features (down in *daf-22*). Isotope and adduct peaks were removed as much as possible at this step. Known ascarosides are included.	245	325	368
Number of differential features that were analyzed by MS/MS (after manual QC to more carefully remove redundant features). Known ascarosides are excluded.	156		
Number of new metabolites (after MS/MS)	96		
Number of detected known ascarosides (out of 19 found by manual analysis).	9	16	13

Table S2. Differential metabolites from *C. elegans* L1 medium, ES- mode, that are decreased or absent in *daf-22* medium compared to N2. Peaks that are present but not differential in growth medium are shown in blue. Peaks that are also differential in growth medium are shown in red. **Peaks that are also in growth medium table (ES-) are shown in bold red.** Manually added entries are shaded pink. Entries that have a corresponding peak in the ES+ table are shaded grey.

class	*smid-db*	*rt (min)*	*m/z (ES-)*	*MS/MS (ES-)*	*m/z (ES+)*	*MS/MS (ES+)*
ascr		1.57	332.17215	73.02831 (C3H5O2-), 86.02363 (C3H4NO2-), 315.14468 (C15H23O7-)	334.18622	88.03985 (C3H6NO2+), 99.08088 (C6H11O+), 186.11247 (C9H16NO3+), 204.12335 (C9H18NO4+), 218.10239 (C9H16NO5+)
ascr	bhas#9	1.62	**263.11389**	59.01257 (C2H3O2-), 73. 02821 (C3H5O2-), 115.03921 (C5H7O3-), 245.10316 (C11H17O6-)	287.11014	157.04724 (C5H10NaO4+)
		2.19	249.09825			
S		3.43	304.08655	63.96117 (SO2-), 74.00575 (C2H4NS-), 84.04430 (C4H6NO-), 113.04218 (C6H9S-), 116.01672 (C4H6NSO-), 128.03465 (C5H6NO3-), 175.04337 (C7H11SO3-), 178.01790 (C5H8NSO4-)	306.10068	84.04497 (C4H6NO+), 88.03983 (C3H6NO2+), 130.04997 (C5H8NO3+)
		3.44	291.14526			
ascr/osas	osas#13	3.46	841.30273	78.95785 (PO3-), 96.96857 (H2PO4-), 152.99545 (C3H6PO5-), 171.00627 (C3H8PO6-), 444.16269 (C16H31NPO11-)	843.31723	126.09169 (C7H12NO+), 144.10194 (C7H14NO2+)
		3.63	212.97305	69.03333 (C4H5O-), 97.02843 (C5H5O2-), 113.02338 (C5H5O3-), 133.00554 (C5H6ClO2-), 141.01881 (C6H5O4-), 176.99593 (C6H6ClO4-)		
ascr		3.66	374.21887	73.02828 (C3H5O2-), 128.07094 (C6H10NO2-), 357.19171 (C18H29O7-)	376.23325	99.08086 (C6H11O+), 130.08635 (C6H12NO2+), 246.16989 (C12H24NO4+)
ascr/osas	osas#92	3.83	679.24982	78.95792 (PO3-), 96.96864 (H2PO4-), 152.99548 (C3H6PO5-), 171.00626 (C3H8PO6-), 214.04912 (C5H13NPO6-), 234. 07750 (C12H12NO4-), 370.12827 (C13H25NPO9-), 444.16376 (C16H31NPO11-), 661.23810 (C28H42N2PO14-)	681.26385	83.04975 (C5H7O+), 126.09148 (C7H12NO+), 136.07576 (C8H10NO+), 144.10199 (C7H14NO2+), 236.09113 (C12H14NO4+), 316.11551 (C10H23NPO8+)
ascr		3.83	333.15628	73.02825 (C3H5O2-), 87.00761 (C3H3O3-), 315.14514 (C15H23O7-)		
ascr/osas	osas#15	3.94	567.25629	73.02833 (C3H5O2-), 86.02363 (C3H4NO2-), 159.06607 (C7H11O4-), 315.14529 (C15H23O7-), 332.17200 (C15H26NO7-)	569.27057	95.04970 (C6H7O+), 99.08087 (C6H11O+), 119.04942 (C8H7O+), 136.07573 (C8H10NO2+), 218.08138 (C12H12NO3+), 236.09196 (C12H14NO4+), 348.14420 (C18H22NO6+)
ascr/osas	osas#91	4.29	561.22314	73.02827 (C3H5O2-), 98.02370 (C4H4NO2-), 99.00785 (C4H3O3-), 107.04919 (C7H7O-), 119.04951 (C8H7O-), 135.04468 (C8H7O2-), 160.09793 (C7H14NO3-), 216.06636 (C12H10NO3-), 234.07727 (C12H12NO4-), 290.16089 (C13H24NO6-)	549.24268	62.06076 (C2H8NO+), 144.10199 (C7H14NO2+), 166.08386 (C7H13NaNO2+), 176.06816 (C8H11NaNO2+), 184.09436 (C7H15NaNO3+), 212.08916 (C8H15NaNO4+), 226.10486 (C9H17NaNO4+), 276.08420 (C12H15NaNO5+), 296.14679 (C13H23NaNO5+)
GPE		4.32	424.07098	78.95785 (PO3-), 96.96861 (H2PO4-), 152.99554 (C3H6PO5-), 171.00618 (C3H8PO6-), 278.08017 (C1oH17NPO6-), 314.05753 (C10H18ClNPO6-), 352.11713 (C13H23NPO8-), 388.09390 (C13H24ClNPO8-)		
ascr/osas		4.32	644.25732	73.02825 (C3H5O2-), 93.03352 (C6H5O-), 98.02369 (C4H4NO2-), 99.04407 (C5H7O2-), 107.04926 (C7H7O-), 119.04942 (C8H7O-), 135.04453 (C8H7O2-), 190.08771 (C11H12NO2-),	528.20850, 510.19763	101.02370 (C4H5O3+), 119.04937 (C8H7O+), 136.07573 (C8H10NO+), 172.07581 (C11H10NO+), 190.12263 (C12H16NO+),

				216.06660 (C12H10NO3-), 234.07715 (C12H12NO4-), 247.11862 (ascr#9), 482.20258 (C23H32NO10-, osas#9)		200.07111 (C12H10NO2+), 218.08116 (C12H12NO3+), 236.09163 (C12H14NO4+), 290.13840 (C16H20NO4+), 348.14407 (C18H22NO6+)
ascr/osas	glosas#91	4.50	644.25732	73.02825 (C3H5O2-), 93.03352 (C6H5O-), 98.02369 (C4H4NO2-), 99.04407 (C5H7O2-), 107.04926 (C7H7O-), 119.04942 (C8H7O-), 133.02867 (C8H5O2-) 190.08771 (C11H12NO2-), 216.06660 (C12H10NO3-), 247.11862 (ascr#9), 464.19177 (C23H30NO9-)	528.20850	
GPE		4.44	396.17993	78.95783 (PO3-), 96.96854 (H2PO4-), 152.99551 (C3H6PO5-), 171.00624 (C3H8PO6-), 322.14288 (C13H25NPO6-)	398.19443	208.16960 (C13H22NO+), 226.18005 (C13H24NO2+)
ascr/osas	glosas#2	4.67	678.25476	98.02370 (C4H4NO2-), 119.04943 (C8H7O-), 135.04457 (C8H7O2-), 216.06665 (C12H10NO3-), 234.07722 (C12H12NO4-)	661.31915	136.07571 (C8H10NO+), 218.08122 (C12H12NO3+), 236.09161 (C12H14NO4+), 348.14410 (C18H22NO6+), 510.19757 (C24H32NO11+)
ascr/osas	glosas#21	4.87	678.25476	216.06665 (C12H10NO3-), 234.07722 (C12H12NO4-)		
ascr	hbas#13	4.73	529.19427	73.02820 (C3H5O2-), 93.03349 (C6H5O-), 137.02362 (C7H5O3-), 367.13962 (C18H23O8-)		
		4.58	319.17623			
ascr		4.88	**383.14798**	78.95792 (PO3-)		
		4.90	448.21921	71.01270 (C3H3O2-), 73.02835 (C3H5O2-), 85.02843 (C4H5O2-), 88.03938 (C3H6NO2-), 99.04420 (C5H7O2-), 127.03946 (C6H7O3-), 146.08189 (C6H12NO3-), 301.12952 (C14H21O7-)	450.23343	
GPE		4.92	340.15329	78.95784 (PO3-), 96.96854 (H2PO4-), 152.99551 (C3H6PO5-), 171.00624 (C3H8PO6-), 266.11627 (C10H21NPO5-)		
ascr	ascr#81	4.94	521.21423	73.02827 (C3H5O2-), 92.04945 (C6H6N-), 128.03458 (C5H6NO3-), 135.05571 (C7H7N2O-), 136.03976 (C7H6NO2-), 161.07162 (C9H9N2O-), 177.10316 (C10H13N2O-), 203.08263 (C11H11N2O2-), 221.09315 (C11H13N2O3-), 392.17169 (C20H26NO7-), 477.22397 (C24H33N2O8-), 503.20401 (C25H31N2O9-)	393.16550	109.06512 (C7H9O+), 120.04458 (C7H6NO+), 246.11237 (C14H16NO3+)
S		5.00	346.13370	63.96117 (SO2-), 73.98494 (C2H2SO-), 84.04433 (C4H6NO-), 99.98527 (C3H2NSO-), 115.00900 (C4H5NSO-), 160.00723 (C5H6NSO3-), 177.01007 (C5H7NSO4-), 185.11824 (C10H17O3-)	348.14753	74.00657 (C2H4NS+), 92.01695 (C2H6NSO+), 120.01160 (C3H6NSO2+), 120.99564 (C3H5SO3+), 138.02191 (C3H8NSO3+), 151.11176 (C10H15O+), 162.02190 (C5H8NSO3+), 169.12224 (C10H17O2+), 180.03244 (C5H10NSO4+)
ascr		5.07	**463.21976**	59.01261 (C2H3O2-), 71.01261 (C3H3O2-), 73.02829 (C3H5O2-), 85.02836 (C4H5O2-), 101.02341 (C4H5O3-), 113.02342 (C5H5O3-)		
		5.11	241.00450	125.06013 (C7H9O2-), 137.00140 (C4H6ClO3-), 157.00751 (C7H6ClO2-), 161.03720 (C7H10ClO2-), 169.05045 (C8H9O4-), 205.02727 (C8H10ClO4-)		
ascr		5.22	465.23486	59.01256 (C2H3O2-), 71.01261 (C3H3O2-), 73.02828 (C3H5O2-), 85.02850 (C4H5O2-), 89.02345 (C3H5O3-), 101.02354 (C4H5O3-), 113.02370 (C5H5O3-), 155.10762 (C9H15O2-), 173.11816 (C9H17O3-), 303.18134 (C15H27O6-, ascr#10)		
GPE		5.25	418.14124	78.95785 (PO3-), 96.96861 (H2PO4-), 152.99548 (C3H6PO5-), 171.00623 (C3H8PO6-), 214.04825 (C5H13NPO6-),		

				308.12650 (C12H23NPO6-), 382.16367 (C15H29NPO8-)		
		5.26	471.18793		490.22928	197.08083 (C10H13O4+), 293.13824 (C16H21O5+)
GPE		5.33	412.21133	78.95782 (PO3-), 96.96856 (H2PO4-), 152.99547 (C3H6PO5-), 171.00623 (C3H8PO6-), 338.17395 (C14H29NPO6-)	414.22583	98.06045 (C5H8NO+), 224.20087 (C14H26NO+), 242.21132 (C14H28NO2+)
GPE		5.49	410.19571	78.95782 (PO3-), 96.96856 (H2PO4-), 152.99547 (C3H6PO5-), 171.00623 (C3H8PO6-)		
ascr/osas	osas#7	5.49	508.21994	73.02835 (C3H5O2-), 98.02373 (C4H4NO2-), 119.04948 (C8H7O-), 135.04462 (C8H7O2-), 216.06659 (C12H10NO3-), 234.07704 (C12H12NO4-), 273.13449 (C13H21O6-, ascr#7)	532.21613	176.06828 (C8H11NaNO2+), 276.08411 (C12H15NaNO5+), 388.13699 (C18H23NaNO7+)
		5.56	273.17120	59.01261 (C2H3O2-), 115.03916 (C5H7O3-), 139.11215 (C9H15O-)		
ascr/osas	osas#1	5.57	510.23538	73.02824 (C3H5O2-), 82.02866 (C4H4NO-); 98.02371 (C4H4NO2-), 99.00780 (C4H3O3-); 119.04945 (C8H7O-), 121.02873 (C7H5O2-); 123.04453 (C7H7O2-), 127.07574 (C7H11O2-), 133.02895 (C8H5O2-), 216.06650 (C12H10NO3-), 234.07719 (C12H12NO4-), 275.14993 (C13H23O6-, ascr#1)	534.23187	176.06828 (C8H11NaNO2+), 276.08411 (C12H15NaNO5+), 388.13699 (C18H23NaNO7+)
GPE		5.59	456.23779	78.95782 (PO3-), 96.96854 (H2PO4-), 152.99553 (C3H6PO5-), 171.00627 (C3H8PO6-), 214.04861 (C5H13NPO6-)	458.25229	86.06060 (C4H8NO+), 268.22699 (C16H30NO2+), 286.23755 (C16H32NO3+)
		5.61	476.25070	71.01267 (C3H3O2-), 99.04410 (C5H7O2-), 127.07557 (C7H11O2-), 146.08179 (C6H12NO3-), 275.15018 (C13H23O6-), 329.16028 (C16H25O7-)	478.26520	90.05545 (C3H8NO2+), 184.09676 (C9H14NO3+), 202.10744 (C9H16NO4+), 220.11797 (C9H18NO5+), 332.17029 (C15H26NO7+)
S		5.64	372.14917	63.96117 (SO2-), 73.98197 (C2H2SO-), 84.04438 (C4H6NO-), 99.98528 (C3H2NSO-), 115.00896 (C4H5NSO-), 160.00719 (C5H6NSO3-), 177.01004 (C5H7NSO4-), 211.13400 (C12H19O3-)	374.16348	74.00655 (C2H4NS+), 120.01163 (C3H6NSO2+), 138.02196 (C3H8NSO3+), 162.02196 (C5H8NSO3+), 180.03249 (C5H10NSO4+)
ascr	nuclas#33, 34	5.75	695.29083	72.00783 (C2H2NO2-), 74.02348 (C2H4NO2-), 100.00296 (C3H2NO3-), 118.05013 (C4H8NO3-), 160.02628 (C6H2N5O-)	697.30518	136.06183 (C5H6N5+), 162.04111 (C6H4N5O+), 281.09924 (C10H13N6O4+), 287.14908 (C14H23O6+)
GPE		5.78	424.21146	78.95782 (PO3-), 96.96854 (H2PO4-), 152.99553 (C3H6PO5-), 171.00633 (C3H8PO6-), 350.17386 (C15H29NPO6-)	426.22596	254.21124 (C15H28NO2+)
		5.79	255.02007	139.07593 (C8H11O2-), 151.01729 (C5H8ClO3-), 175.05299 (C8H12ClO2-), 219.04298 (C9H12ClO4-)		
GPE		5.80	426.22705	78.95780 (PO3-), 96.96851 (H2PO4-), 152.99542 (C3H6PO5-), 171.00615 (C3H8PO6-), 352.18945 (C15H31NPO6-)	428.24146	256.22733 (C15H30NO2+)
ascr/osas	glosas#10	5.78	700.32025	73.02825 (C3H5O2-), 82.02863 (C4H4NO2-), 123.04437 (C7H7O2-), 133.02884 (C8H5O2-), 155.10735 (C9H15O2-), 173.11801 (C9H17O3-), 216.06662 (C12H10NO3-), 303.18134 (C15H27O6-, ascr#10), 520.25446 (C27H38NO9-)	528.20850, 510.19763	72.08144 (C4H10N+), 119.04937 (C8H7O+), 136.07570 (C8H10NO+), 218.08116 (C12H12NO3+), 236.09167 (C12H14NO4+), 348.14368 (C18H22NO6+)
ascr/osas	glosas#101	5.92	700.32025	73.02825 (C3H5O2-), 82.02863 (C4H4NO2-), 123.04437 (C7H7O2-), 133.02884 (C8H5O2-), 155.10735 (C9H15O2-), 173.11801 (C9H17O3-), 216.06662 (C12H10NO3-), 303.18134 (C15H27O6-, ascr#10), 520.25446 (C27H38NO9-)	528.20850	
GPE		5.87	504.23795	78.95781 (PO3-), 96.96851 (H2PO4-), 140.01126 (C2H7NPO4-), 152.99548 (C3H6PO5-), 171.00618 (C3H8PO6-), 214.04874 (C5H13NPO6-)	506.25245	334.23740 (C20H32NO3+)
ascr/osas	osas#22	5.89	550.16319	98.02370 (C4H4NO2-), 99.00771 (C4H3O3-); 119.04945 (C8H7O-),	498.18970	136.07576 (C8H10NO+), 218.08125 (C12H12NO3+),

				121.02872 (C7H5O2-); 135.04451 (C8H7O2-), 190.08725 (C11H12NO2-); 216.06657 (C12H10NO3-), 234.07710 (C12H12NO4-)		236.09166 (C12H14NO4+), 348.14420 (C18H22NO6+),
		5.93	239.02522			
S		6.06	343.13391		345.14813	58.99575 (C2H3S+), 104.01679 (C3H6NSO+), 116.01688 (C4H6NSO+), 140.05286 (C7H10NS+), 168.04774 (C8H10NSO+), 172.07903 (C8H14NSO+), 196.04274 (C9H10NSO2+), 281.13171 (C14H21N2SO2+), 299.14227 (C14H23N2SO3+), 327.13712 (C15H23N2SO4+)
GPE		6.11	442.14105	78.95782 (PO3-), 96.96853 (H2PO4-), 140.01122 (C2H7NPO4-), 152.99548 (C3H6PO5-), 171.00616 (C3H8PO6-), 214.04875 (C5H13NPO6-), 388.15372 (C17H27NPO7-), 406.16357 (C17H29NPO8-)	444.15555	272.14105 (C14H23O2NCl+)
		6.18	301.20261	99.08054 (C6H11O-), 139.11227 (C9H15O-), 143.07088 (C7H11O3-), 183.10243 (C10H15O3-), 201.11340 (C10H17O4-)		
GPE		6.20	452.10220	78.95783 (PO3-), 96.96857 (H2PO4-), 140.01120 (C2H7NPO4-), 152.99547 (C3H6PO5-), 171.00627 (C3H8PO6-), 214.04877 (C5H13NPO6-), 380.14795 (C15H27NPO8-), 416.12509 (C15H28ClNPO8-)		
GPE		6.21	452.24268	78.95781 (PO3-), 96.96851 (H2PO4-), 152.99544 (C3H6PO5-), 171.00615 (C3H8PO6-)	454.25718	282.24265 (C17H32NO2+)
GPE		6.22	440.24258	78.95781 (PO3-), 96.96853 (H2PO4-), 152.99544 (C3H6PO5-), 171.00618 (C3H8PO6-), 366.20477 (C16H33NPO6-)	442.25708	98.06040 (C5H8NO+), 252.23201 (C16H30NO+), 270.24255 (C16H32NO2+)
GPE		6.23	446.17233	78.95784 (PO3-), 96.96852 (H2PO4-), 152.99541 (C3H6PO5-), 171.00616 (C3H8PO6-), 336.15781 (C14H27NPO6-), 410.19498 (C17H33NPO8-)		
GPE		6.28	434.09137	78.95788 (PO3-), 152.99577 (C3H6PO5-), 171.00594 (C3H8PO6-), 362.13797 (C15H25NPO7-), 398.11340 (C15H26ClNPO7-)		
GPE		6.35	544.25366	59.01267 (C2H3O2-), 71.01264 (C3H3O2-), 78.95789 (PO3-), 85.02838 (C4H5O2-), 89.02330 (C3H5O3-), 96.96855 (H2PO4-), 101.02345 (C4H5O3-), 113.02343 (C5H5O3-), 119.03423 (C4H7O4-), 152.99577 (C3H6PO5-), 333.05933 (C9H18PO11-)	546.26816	212.20088 (C13H26NO+)
GPE		6.41	**368.18481**	78.95782 (PO3-), 96.96851 (H2PO4-), 152.99545 (C3H6PO5-), 171.00621 (C3H8PO6-), 294.14777 (C12H25NPO5-)	370.19931	198.18527 (C12H24NO+)
sulfate		6.42	281.14310	96.95911 (HSO4-)		
GPE		6.43	380.18481	78.95786 (PO3-), 96.96860 (H2PO4-), 152.99556 (C3H6PO5-), 171.00627 (C3H8PO6-), 306.14774 (C13H25NPO5-)	382.19931	210.18518 (C13H24NO+)
		6.45	**225.11349**	163.11259 (C11H15O-), 181.12340 (C11H17O2-)		
		6.46	470.21649	78.95783 (PO3-), 96.96856 (H2PO4-), 259.02261 (C6H12PO9-), 308.16348 (C13H27NPO5-)		
sulfate		6.59	279.12747	96.95911 (HSO4-)		
		6.70	227.12935	97.06491 (C6H9O-), 165.12825 (C11H17O-), 183.13882 (C11H19O2-), 209.11833 (C12H17O3-)		
GPE		6.72	382.20074	78.95795 (PO3-), 96.96865 (H2PO4-), 152.99550 (C3H6PO5-), 171.00623 (C3H8PO6-), 308.16330 (C13H27NPO5-)	384.21524	212.20082 (C13H26NO+)

GPE		6.75	436.10703	78.95782 (PO3-), 96.96848 (H2PO4-), 152.99545 (C3H6PO5-), 171.00623 (C3H8PO6-), 290.11664 (C12H21NPO5-), 364.15302 (C15H27NPO7-), 400.12967 (C15H28ClNPO7-)	438.12153	194.15393 (C12H20NO+), 266.10703 (C12H22ONCl2+)
GPE		6.76	462.22723	78.95785 (PO3-), 96.96857 (H2PO4-), 152.99561 (C3H6PO5-), 171.00629 (C3H8PO6-)	464.24173	274.21619 (C18H28NO+), 292.22681 (C18H30NO2+)
GPE		6.94	472.18796	78.95782 (PO3-), 96.96861 (H2PO4-), 152.99547 (C3H6PO5-), 171.00626 (C3H8PO6-), 436.21048 (C19H35NPO8-)	474.20246	248.20082 (C16H26NO+), 266.21118 (C16H28NO2+), 302.18796 (C16H29ClNO2+)
GPE		7.14	**582.26947**	59.01256 (C2H3O2-), 71.01260 (C3H3O2-), 78.95783 (PO3-), 89.02332 (C3H5O3-), 96.96854 (H2PO4-), 101.02341 (C4H5O3-), 113.02357 (C5H5O3-), 119.03416 (C4H7O4-), 152.99548 (C3H6PO5-), 171.00616 (C3H8PO6-), 333.05972 (C9H18PO11-)	584.28397	250.21646 (C16H28NO+)
GPE		7.28	**606.26965**	59.01256 (C2H3O2-), 71.01258 (C3H3O2-), 78.95782 (PO3-), 89.02328 (C3H5O3-), 96.96855 (H2PO4-), 101.02338 (C4H5O3-), 113.02349 (C5H5O3-), 119.03416 (C4H7O4-), 152.99548 (C3H6PO5-), 171.00626 (C3H8PO6-), 333.05948 (C9H18PO11-)	608.28415	274.21637 (C18H28NO+)
		7.42	532.23260	78.95787 (PO3-), 96.96854 (H2PO4-), 370.17862 (C18H29NPO5-)		
GPE		7.44	474.20380	78.95783 (PO3-), 96.96849 (H2PO4-), 152.99550 (C3H6PO5-), 171.00621 (C3H8PO6-), 438.22610 (C19H37NPO8-)		
GPE		7.52	608.28552	59.01255 (C2H3O2-), 71.01257 (C3H3O2-), 78.95782 (PO3-), 85.02837 (C4H5O2-), 89.02325 (C3H5O3-), 96.96856 (H2PO4-), 101.02342 (C4H5O3-), 113.02359 (C5H5O3-), 119.03427 (C4H7O4-), 152.99542 (C3H6PO5-), 171.00644 (C3H8PO6-), 333.05966 (C9H18PO11-)		
GPE		7.53	**596.28528**	59.01256 (C2H3O2-), 71.01261 (C3H3O2-), 78.95783 (PO3-), 89.02332 (C3H5O3-), 96.96854 (H2PO4-), 101.02345 (C4H5O3-), 152.99550 (C3H6PO5-), 333.06049 (C9H18PO11-)	598.29978	264.23196 (C17H30NO+)
EA		7.67	280.16898		246.20680	
GPE		7.86	**632.28528**	59.01255 (C2H3O2-), 71.01259 (C3H3O2-), 78.95781 (PO3-), 89.02328 (C3H5O3-), 96.96852 (H2PO4-), 101.02338 (C4H5O3-), 113.02361 (C5H5O3-), 119.03419 (C4H7O4-), 140.01123 (C2H7NPO4-), 152.99545 (C3H6PO5-), 171.00592 (C3H8PO6-), 196.03804 (C5H11NPO5-), 214.04857 (C5H13NPO6-), 333.05920 (C9H18PO11-), 376.10150 (C11H23NPO11-)	634.29950	300.23224 (C20H30NO+)
GPE		8.04	**610.30066**	59.01258 (C2H3O2-), 71.01263 (C3H3O2-), 78.95790 (PO3-), 89.02340 (C3H5O3-), 96.96866 (H2PO4-), 101.02349 (C4H5O3-), 113.02362 (C5H5O3-), 119.03426 (C4H7O4-), 152.99551 (C3H6PO5-), 171.00633 (C3H8PO6-), 333.05917 (C9H18PO11-)	612.31439	278.24771 (C18H32NO+)
GPE		8.10	**598.30084**	59.01257 (C2H3O2-), 71.01258 (C3H3O2-), 78.95782 (PO3-), 89.02328 (C3H5O3-), 96.96854 (H2PO4-), 101.02338 (C4H5O3-), 113.02354 (C5H5O3-), 119.03410 (C4H7O4-), 152.99547 (C3H6PO5-), 171.00618 (C3H8PO6-), 333.05948 (C9H18PO11-)	600.31488	98.06043 (C5H8NO+), 266.24771 (C17H32NO+)

Table S3. Differential metabolites from *C. elegans* growth medium, ES- mode, that are decreased or absent in *daf-22* medium compared to N2. Peaks that are present but not differential in L1 medium are shown in blue. Peaks that are also differential in L1 medium are shown in red. **Peaks that are also in L1 medium table (ES-) are shown in bold red.** Manually added entries are shaded pink. Entries that have a corresponding peak in the ES+ table are shaded grey.

class	*smid-db*	*rt (min)*	*m/z (ES-)*	*MS/MS (ES-)*	*m/z (ES+)*	*MS/MS (ES+)*
ascr	bhas#9	1.79	**263.11383**	59.01257 (C2H3O2-), 73. 02821 (C3H5O2-), 115.03921 (C5H7O3-), 245.10316 (C11H17O6-)	287.11014	157.04724 (C5H10NaO4+)
ascr	uglas#11	2.92	667.18811	78.95777 (PO3-), 96.96848 (H2PO4-), 124.01446 (C4H2N3O2-), 167.02077 (C5H3N4O3-), 178.02559 (C7H4N3O3-), 223.00130 (C6H8PO7-), 241.01166 (C6H10PO8-), 275.14966 (C13H23O6-, ascr#1), 293.05246 (C11H9N4O6-), 311.06277 (C11H11N4O7-), 391.02945 (C11H12N4PO10-), 409.03973 (C11H14N4PO11), 499.15857 (C19H32PO13-), 537.12195 (C18H26N4PO13-), 569.21106 (C24H33N4O12-), 624.17889 (C23H35N3PO15-)	669.20190, 539.13904	98.98456 (H4PO4+), 97.02879 (C5H5O2+), 127.03919 (C6H7O3+), 129.09111 (C7H13O2+), 169.03543 (C5H5N4O3+), 243.02618 (C6H12PO8+)
ascr	uglas#1	3.70	587.22061			
		3.74	427.13766			
ascr		3.83	517.16962	78.95777 (PO3-), 96.96849 (H2PO4-), 241.01221 (C6H10PO8-)		
		3.84	723.21429	78.95778 (PO3-), 96.96848 (H2PO4-), 114.05506, 128.03453, 167.02094 (C5H3N4O3-), 178.02570 (C7H4N3O3-)		
ascr		3.87	355.11676	78.95777 (PO3-)		
		3.89	241.02739		243.04189	
		4.31	923.31970	78.95778 (PO3-), 167.02072 (C5H3N4O3-),		
ascr		4.46	749.22992	78.95776 (PO3-), 96.96847 (H2PO4-), 102.05496 (C4H8NO2-), 124.01448 (C4H2N3O2-), 128.03450 (C5H6NO3-), 167.02075 (C5H3N4O3-), 178.02559 (C7H4N3O3-), 186.12457 (C8H16N3O2-), 208.10902 (C10H14N3O2-), 227.10361 (C10H15N2O4-), 393.10526 (C16H17N4O8-), 470.29791, 491.08157, 581.20013	621.18109	97.02879 (C5H5O2+), 98.98442 (H4PO4+), 127.03907 (C6H7O3+), 129.09117 (C7H13O2+), 167.08168 (C8H11N2O2+), 169.03531 (C5H5N4O3+), 209.0808 (C11H13O4+), 219.14922 (C13H19N2O+), 227.09126 (C11H15O5+), 229.15456 (C11H21N2O3+), 300.15515 (C13H22N3O5+), 307.05759 (C11H16PO8+), 337.16360 (C12H26N4PO5+), 341.18253 (C15H25N4O5+), 342.23871 (C17H32N3O4+), 362.17044 (C18H24N3O5+)
		4.55	751.24493	78.95777 (PO3-), 96.96848 (H2PO4-), 124.01422 (C4H2N3O2-), 127.05039 (C5H7N2O2-), 128.03445 (C5H6NO3-), 167.02060 (C5H3N4O3-), 178.02544 (C7H4N3O3-), 493.09698, 583.21722 (?)		
		4.64	785.22943	78.95777 (PO3-), 124.01422 (C4H2N3O2-), 167.02060 (C5H3N4O3-)		
ascr		4.64	381.13177	78.95776 (PO3-)	211.03685	
ascr	ascr#82	4.76	650.25781	73.02825 (C3H5O2-), 92.04943 (C6H6N-), 102.05498 (C4H8NO2-), 128.03450 (C5H6NO3-), 146.04530 (C5H8NO4-), 203.08250 (C11H11N2O2-), 221.09302 (C11H13N2O3-), 392.17139	652.27191	120.04460 (C7H6NO+), 246.11238 (C14H16NO3+)

				(C20H26NO7-, ascr#8), 503.20291 (C25H31N2O9-), 521.21362 (C25H33N2O10-), 632.24597 (C30H38N3O12-)		
		4.80	599.21228	78.95778 (PO3-), 96.96848 (H2PO4-)		
ascr		4.81	**383.14828**	78.95792 (PO3-)		
		4.82	604.18127	78.95778 (PO3-), 96.96849 (H2PO4-), 114.05508 (C5H8NO2-), 127.05049 (C5H7N2O2- ?), 129.10262 (C6H13N2O- ?), 131.04538 (C4H7N2O3- ?), 240.13531 (C11H18N3O3- ?), 258.14575 (C11H20N3O4- ?)	606.19577	
ascr		4.85	574.17072	78.95778 (PO3-), 96.96848 (H2PO4-), 358.07004 (C14H17NPO8-)	576.18439	87.04459 (C4H7O2+), 95.04962 (C6H7O+), 98.98460 (H4PO4+), 118.06536 (C8H8N+), 127.03914 (C6H7O3+), 158.06021 (C10H8NO+), 172.07562 (C11H10NO+), 226.08620 (C14H12NO2+), 243.02664 (C6H12PO8+), 244.09686 (C14H14NO3+), 458.12155 (C19H25NPO10+)
		4.88	951.35046	78.95779 (PO3-), 96.96850 (H2PO4-), 124.01435 (C4H2N3O2-), 167.02072 (C5H3N4O3-), 178.02536 (C7H4N3O3-), 675.19305, 693.20465, 783.32550	953.36496	127.03922 (C6H7O3+), 137.09625 (C9H13O+), 281.13837 (C15H21O5+), 675.22778
ascr	uglas#3	4.92	613.23743	84.00776 (C3H2NO2-), 99.01884 (C3H3N2O2-), 124.01435 (C4H2N3O2-), 141.02994 (C5H5N2O3-), 167.02077 (C5H3N4O3-), 180.04128 (C7H6N3O3-), 268.05731 (C10H10N3O6-), 311.06326 (C11H11N4O7-)	615.25193	127.03912 (C6H7O3+), 137.09621 (C9H13O+), 155.10675 (C9H15O2+), 169.03560 (C5H5N4O3+), 173.11771 (C9H17O3+), 187.10759 (C8H15N2O3+), 215.10280 (C9H15N2O4+), 281.13821 (C15H21O5+), 299.14908 (C15H23O6+), 317.16000 (C15H25O7+), 328.18646 (C15H26N3O5+), 441.27097 (C21H37N4O6+), 467.17691 (C20H27N4O9+)
ascr		4.95	638.23297	71.01260 (C3H3O2-), 107.03544 (C4H3N4-), 115.00285 (C4H3O4-), 134.04654 (C5H4N5-), 162.07819 (C7H8N5-), 188.05774 (C8H6N5O-), 206.06824 (C8H8N5O2-)	640.24683	129.10226 (C6H13N2O+), 136.06172 (C5H6N5+), 162.07738 (C7H8N5+), 188.05649 (C8H6N5O+), 192.05151 (C7H6N5O2+), 206.06705 (C8H8N5O2+), 234.06195 (C9H8N5O3+), 252.07259 (C9H10N5O4+), 259.11755 (C12H19O6+), 510.18301 (C21H28N5O10+)
ascr		5.03	792.27258	78.95776 (PO3-), 96.96846 (H2PO4-)	794.28632	136.06175 (C5H6N5+), 148.06194 (C6H6N5+), 262.09311 (C11H12N5O3+), 287.14896 (C14H23O6+), 378.08072 (C11H17N5PO8+)
ascr		5.05	640.24872		642.26322	136.06180 (C5H6N5+), 162.07738 (C7H8N5+), 252.07251 (C9H10N5O4+), 359.17099 (C18H23N4O4+), 428.25092 (C19H34N5O6+), 512.19836 (C21H30N5O10+)
ascr		5.06	**463.21936**	59.01253 (C2H3O2-), 71.01257 (C3H3O2-), 73.02823 (C3H5O2-), 85.02837 (C4H5O2-), 101.02341 (C4H5O3-), 113.02359 (C5H5O3-)	482.26001	
ascr		5.06	560.15472	78.95789 (PO3-), 96.96860 (H2PO4-), 412.08038 (C17H19NPO9-)	562.16922	127.03913 (C6H7O3+), 130.06519 (C9H8N+), 444.10501 (C18H23NPO10+)
EA		5.15	256.15598		258.17048	152.10698 (C9H14NO+), 194.11757 (C11H16NO2+), 212.12811 (C11H18NO3+), 222.11237 (C12H16NO3+), 240.15915 (C13H22NO3+)
		5.16	632.21271	78.95776 (PO3-), 96.96848 (H2PO4-)	634.22721	
		5.21	497.09778	78.95779 (PO3-), 96.96851 (H2PO4-)	499.11228	
		5.22	564.18628			
ascr		5.28	435.22433	59.01256 (C2H3O2-), 73.02819		

				(C3H5O2-), 85.02831 (C4H5O2-), 111.04420 (C6H7O2-), 113.02335 (C5H5O3-), 155.10727 (C9H15O2-), 173.11801 (C9H17O3-), 287.15033 (C14H23O6-), 305.16031 (C14H25O7-)		
		5.31	634.19214	78.95776 (PO3-), 96.96851 (H2PO4-), 223.00159 (C6H8PO7-), 497.14322 (C19H30PO13-)	636.20664	109.06512 (C7H9O+), 120.04447 (C7H6NO+), 127.07549 (C7H11O2+)
		5.34	630.19720	78.95778 (PO3-), 96.96852 (H2PO4-)	632.21170	
		5.37	350.17453	78.95783 (PO3-), 96.96857 (H2PO4-), 140.01125 (C2H7NPO4-)	352.18903	98.06043 (C5H8NO+), 236.20067 (C15H26NO+), 254.21118 (C15H28NO2+)
ascr	iglas#91	5.37	588.18646	78.95776 (PO3-), 96.96845 (H2PO4-)	590.20096	98.98453 (H4PO4+), 101.06011 (C5H9O2+), 118.06529 (C8H8N+), 127.03906 (C6H7O3+), 130.06509 (C9H8N+), 158.06007 (C10H8NO+), 226.08649 (C14H12NO2+), 244.09703 (C14H14NO3+), 256.22672 (C15H30NO2+), 362.15912 (C19H24NO6+), 472.13617 (C10H27NPO10+)
		5.42	779.27753	78.95778 (PO3-), 96.96849 (H2PO4-), 167.02077 (C5H3N4O3-)		
ascr	iglas#11 (2nd peak)	5.44	616.21698	78.95778 (PO3-), 96.96849 (H2PO4-), 2nd peak also has 340.05902 (C14H15NPO6-), 358.06961 (C14H17NPO8-)	488.16867, 618.23224	98.98457 (H4PO4+), 109.02872 (C6H5O2+), 118.06540 (C8H8N+), 127.03906 (C6H7O3+), 129.09109 (C7H13O2+), 154.06520 (C11H8N+), 158.05997 (C10H8NO+), 180.08072 (C13H10N+), 184.07574 (C12H10NO+), 198.09140 (C13H12NO+), 202.08638 (C12H12NO2+), 210.09100 (C14H12NO+), 226.08617 (C14H12NO2+), 237.11197 (C13H17O4+), 244.09689 (C14H14NO3+), 255.12274 (C13H19O5+), 262.10727 (C14H16NO4+), 335.08871 (C13H20PO8+), 354.16925 (C21H24NO4+), 372.18027 (C21H26NO5+), 390.19098 (C21H28NO6+)
		5.48	585.15051	92.04934 (C6H6N-), 116.04958 (C8H6N-), 136.03961 (C7H6NO2-), 160.03989 (C9H6NO2-), 172.04019 (C10H6NO2-), 178.05067 (C9H8NO3-), 190.05072 (C10H8NO3-), 250.07254 (C12H12NO5-), 268.08231 (C12H14NO6-), 412.12393 (C18H22NO10-)	551.18833	73.02906 (C3H5O2+), 85.02896 (C4H5O2+), 92.04992 (C6H6N+), 97.02882 (C5H5O2+), 120.04457 (C7H6NO+), 132.04445 (C8H6NO+), 134.06006 (C8H8NO+), 162.05481 (C9H8NO2+), 170.06010 (C11H8NO+), 180.06534 (C9H10NO3+), 198.05493 (C12H8NO2+), 216.06552 (C12H10NO3+), 234.07622 (C12H12NO4+), 252.08681 (C12H14NO5+), 270.09680 (C12H16NO6+), 282.09695 (C13H16NO6+), 378.11761 (C18H20NO8+), 396.12863 (C18H22NO9+)
ascr		5.50	455.20572	78.95777 (PO3-), 96.96849 (H2PO4-), 209.02197 (C6H10PO6-)	457.22022	
		5.52	285.17117	87.04401 (C4H7O2-), 115.07559 (C6H11O2-), 125.09640 (C8H13O-), 143.06897 (C7H11O3-), 155.10735 (C9H15O2-), 169.12308 (C19H17O2-), 241.18080 (C14H25O3-)	309.16757	291.15640 (C15H24NaO4+)
		5.52	530.18048			
		5.58	602.20239		604.21689	
ascr	nuclas#35, 36	5.65	666.26398	71.01255 (C3H3O2-), 107.03518 (C4H3N4-), 115.00274 (C4H3O4-), 134.04639 (C5H4N5-), 162.07800 (C7H8N5-), 188.05809 (C8H6N5O-), 206.06813 (C8H8N5O2-), 250.05795 (C9H8N5O4-), 338.11041 (C13H16N5O6-),	668.27832	113.05988 (C6H9O2+), 136.06180 (C5H6N5+), 148.06177 (C6H6N5+), 155.10663 (C9H15O2+), 162.07733 (C7H8N5+), 173.11732 (C9H17O3+), 188.05664 (C8H6N5O+), 192.05151 (C7H6N5O2+), 206.06723 (C8H8N5O2+), 234.06197 (C9H8N5O3+), 252.07254

				382.10068 (C14H16N5O8-)		(C9H10N5O4+), 287.14871 (C14H23O6+), 382.13580 (C15H20N5O7+), 417.21103 (C20H33O9), 538.21429 (C23H32N5O10+)
ascr		5.67	411.17960	78.95777 (PO3-), 96.96845 (H2PO4-)	413.19410	83.04971 (C5H7O+), 95.04955 (C6H7O+), 113.05999 (C6H9O2+), 149.13264 (C11H17+), 167.14304 (C11H19O2+), 185.15347 (C11H21O2+), 211.03659 (C6H12PO6+)
ascr	anglas#7	5.70	590.20203	92.04940 (C6H6N-), 136.03970 (C7H6NO2-), 453.15356 (C19H30ClO10-)	556.23993	95.04960 (C6H7O+), 109.06513 (C7H9O+), 113.05999 (C6H9O2+), 120.04459 (C7H6NO+), 127.07548 (C7H11O2+), 138.05496 (C7H8NO2+), 146.02361 (C8H4NO2+), 162.05519 (C9H8NO2+), 172.07555 (C11H10NO+), 180.06519 (C9H10NO3+), 186.05501 (C11H8NO2+), 210.05490 (C13H8NO2+), 228.06540 (C13H10NO3+), 246.07628 (C13H12NO4+), 250.10721 (C13H16NO4+), 268.11755 (C13H18NO5+), 271.11731 (C13H19O6+), 289.12814 (C13H21O7+), 372.14462 (C20H22NO6+), 390.15500 (C20H24NO7+), 408.16544 (C20H26NO8+), 426.17566 (C20H28NO9+)
ascr	iglas#71	5.70	614.20160	78.95777 (PO3-), 96.96847 (H2PO4-), 358.06989 (C14H17NPO8-)	616.21661	109.06519 (C7H9O+), 118.06535 (C8H8N+), 127.03898 (C6H7O3+), 127.07549 (C7H11O2+), 130.06525 (C9H8N+), 144.08086 (C10H10N+), 172.07538 (C11H10NO+), 226.08644 (C14H12NO2+), 235.09691 (C13H15O4+), 243.02646 (C6H12PO8+), 244.09651 (C14H14NO3+), 262.10687 (C14H16NO4+), 370.16519 (C21H24NO5+), 388.17554 (C21H26NO6+)
		5.76	334.17972		300.21729	
ascr		5.78	544.19635	73.02822 (C3H5O2-), 116.04964 (C8H6N-), 247.11865 (C11H19O6-, ascr#9), 278.10324 (C14H16NO5-)		
ascr	anglas#1	5.79	592.21759	92.04939 (C6H6N-), 136.03969 (C7H6NO2-), 455.16901 (C19H32ClO10-)	558.25586	95.04960 (C6H7O+), 111.08076 (C7H11O+), 113.06001 (C6H9O2+), 120.04460 (C7H6NO+), 129.09111 (C7H13O2+), 138.05499 (C7H8NO2+), 146.02357 (C8H4NO2+), 162.05463 (C9H8NO2+), 172.07555 (C11H10NO+), 180.06555 (C9H10NO3+), 228.06544 (C13H10NO3+), 237.11195 (C13H17O4+), 250.10730 (C13H16NO4+), 255.12253 (C13H19O5+), 268.11777 (C13H18NO5+), 273.13324 (C13H21O6+), 374.15930 (C20H24NO6+), 392.17081 (C20H26NO7+), 410.181184 (C20H28NO8+), 428.19128 (C20H30NO9+)
GPE		5.80	412.21088	78.95777 (PO3-), 96.96841 (H2PO4-), 152.99530 (C3H6PO5-), 171.00607 (C3H8PO6-)	414.22538	98.06047 (C5H8NO+), 224.20096 (C14H26NO+), 242.21140 (C14H28NO2+)
ascr		5.88	409.16388	78.95780 (PO3-), 96.96854 (H2PO4-)	411.17838	83.04975 (C5H7O+), 95.04975 (C6H7O+), 113.06001 (C6H9O2+), 137.09607 (C9H13O+), 183.13815 (C11H19O2+), 201.14886 (C11H21O3+), 211.03673 (C6H12PO6+)
EA		5.98	310.17966		276.21748	62.06081 (C2H8NO+), 240.19566 (C14H26NO2+), 258.20624 (C14H28NO3+)
GPE		6.03	438.22690	78.95776 (PO3-), 96.96840 (H2PO4-), 152.99524 (C3H6PO5-), 171.00600 (C3H8PO6-), 364.18936 (C16H31NPO6-)	440.24140	250.21649 (C16H28NO+), 268.22696 (C16H30NO2+)
GPE		6.10	**368.18478**	78.95783 (PO3-), 96.96849	370.19928	198.18520 (C12H24NO+)

				(H2PO4-), 152.99535 (C3H6PO5-), 171.00609 (C3H8PO6-), 294.14722 (C12H25NPO5-)		
ascr	iglas#7	6.17	570.21198	73.02822 (C3H5O2-), 83.04903 (C5H7O-), 101.02339 (C4H5O3-), 111.04424 (C6H7O2-), 116.04966 (C8H6N-), 125.06000 (C7H9O2-), 273.13434 (C13H21O6-, ascr#7), 278.10318 (C14H16NO5-)	536.24980	127.07551 (C7H11O2+), 130.06526 (C9H8N+), 230.11761 (C14H16NO2+), 254.11775 (C16H16NO2+), 289.12820 (C13H21O7+)
		6.17	378.20551	78.95777 (PO3-), 96.96846 (H2PO4-), 140.01117 (C2H7NPO4-)	380.22001	98.06042 (C5H8NO+), 264.23199 (C17H30NO+), 282.24255 (C17H32NO2+)
ascr	iglas#31	6.26	642.23291	78.95786 (PO3-), 96.96859 (H2PO4-), 358.06979 (C14H17NPO8-)	644.24701	118.06532 (C8H8N+), 127.03913 (C6H7O3+), 130.06526 (C9H8N+), 137.09615 (C9H13O+), 226.08643 (C14H12NO2+), 281.13889 (C15H21O5+), 398.19626 (C23H28NO5+), 416.20734 (C23H30NO6+)
ascr	iglas#1	6.30	572.22729	73.02820 (C3H5O2-), 116.04965 (C8H6N-), 127.07566 (C7H11O2-), 275.14975 (C13H23O6-, ascr#1), 278.10309 (C14H16NO5-)	538.26520	95.04958 (C6H7O+), 111.08086 (C7H11O+), 118.06535 (C8H8N+), 130.06519 (C9H8N+), 144.08075 (C10H0N+), 158.06001 (C10H8NO+), 172.07564 (C11H10NO+), 184.07570 (C12H10NO+), 184.11212 (C13H14N+), 212.10701 (C14H14NO+), 230.11742 (C14H16NO2+), 254.11760 (C16H16NO2+), 272.12784 (C16H18NO3+), 484.23303 (C27H34NO7+)
GPE		6.34	580.25354	59.01253 (C2H3O2-), 71.01254 (C3H3O2-), 78.95779 (PO3-), 89.02324 (C3H5O3-), 96.96848 (H2PO4-), 101.02332 (C4H5O3-), 113.02347 (C5H5O3-), 119.03403 (C4H7O4-), 152.99541 (C3H6PO5-), 171.00626 (C3H8PO6-), 333.05923 (C9H18PO11-)	582.26804	248.20082 (C16H26NO+)
		6.38	453.10767	92.04941 (C6H6N-), 116.04967 (C8H6N-), 136.03972 (C7H6NO2-), 178.05064 (C9H8NO3-)	419.14514	95.04994 (C6H6N+), 120.04459 (C7H6NO+), 97.02884 (C5H5O2+), 138.05496 (C7H8NO2+), 228.06548 (C13H10NO3+), 264.08649 (C14H14NO5+), 282.09708 (C13H16NO6+)
		6.39	**225.11357**	59.01254 (C2H3O2-), 163.11240 (C11H15O-), 181.12320 (C11H17O2-)		
GPE		6.66	570.26923	59.01252 (C2H3O2-), 71.01255 (C3H3O2-), 78.95779 (PO3-), 89.02321 (C3H5O3-), 96.96848 (H2PO4-), 101.02333 (C4H5O3-), 113.02354 (C5H5O3-), 119.03412 (C4H7O4-), 152.99535 (C3H6PO5-), 171.00612 (C3H8PO6-), 333.05914 (C9H18PO11-)	572.28406	98.06041 (C5H8NO+), 112.07590 (C6H10NO+), 126.09136 (C7H12NO), 140.10696 (C8H14NO+), 238.21637 (C15H28NO+), 256.22693 (C15H30NO2+), 410.22925 (C18H37NPO7+)
GPE		6.68	**582.26923**	59.01254 (C2H3O2-), 71.01256 (C3H3O2-), 78.95779 (PO3-), 89.02323 (C3H5O3-), 96.96850 (H2PO4-), 101.02335 (C4H5O3-), 113.02353 (C5H5O3-), 119.03412 (C4H7O4-), 152.99547 (C3H6PO5-), 171.00610 (C3H8PO6-), 333.05923 (C9H18PO11-)	584.28400	250.21646 (C16H28NO+)
GPE		6.73	594.26929	59.01254 (C2H3O2-), 71.01251 (C3H3O2-), 78.95778 (PO3-), 89.02315 (C3H5O3-), 96.96845 (H2PO4-), 101.02335 (C4H5O3-), 152.99541 (C3H6PO5-)	596.28379	262.21640 (C17H28NO+)
		6.76	496.23230	78.95782 (PO3-), 96.96849 (H2PO4-), 138.97931 (C2H4PO5-), 140.01134 (C2H7NPO4-), 259.02188 (C6H12PO9-), 316.16827 (C15H27NPO4-), 334.17877 (C15H29NPO5-),		

				376.18976 (C17H31NPO6-)		
EA		6.78	292.16898	86.02374 (C3H4NO2-), 142.08717 (C7H12NO2-), 256.19217 (C14H26NO3-)	258.20651	62.06083 (C2H8NO+), 70.02945 (C3H4NO+), 88.03984 (C3H6NO2+), 128.07065 (C6H10NO2+), 179.14307 (C12H19O+), 198.18536 (C12H24NO+), 222.18533 (C14H24NO+), 240.19576 (C14H26NO2+)
ascr		6.83	598.24384	301.16507 (C15H25O6-, ascr#3)	581.30774	118.06526 (C8H8N+), 130.06512 (C9H8N+), 137.09599 (C9H13O+), 144.08081 (C10H10N+), 155.10666 (C9H15O2+), 160.07570 (C10H10NO+), 170.09636 (C12H12N+), 172.07545 (C11H10NO+), 198.09128 (C13H12NO+), 212.10680 (C14H14NO+), 226.08607 (C14H12NO2+), 317.15897 (C15H25O7+), 398.19669 (C23H28NO5+)
GPE		6.83	**606.26935**	59.01252 (C2H3O2-), 71.01254 (C3H3O2-), 78.95778 (PO3-), 89.02322 (C3H5O3-), 96.96848 (H2PO4-), 101.02332 (C4H5O3-), 113.02352 (C5H5O3-), 119.03402 (C4H7O4-), 152.99533 (C3H6PO5-), 171.00616 (C3H8PO6-), 333.05927 (C9H18PO11-)	608.28345	274.21634 (C18H28NO+)
EA		6.86	294.18445		260.22202	62.06082 (C2H8NO+)
GPE		6.93	618.26941	59.01254 (C2H3O2-), 71.01257 (C3H3O2-), 78.95786 (PO3-), 89.02338 (C3H5O3-), 96.96867 (H2PO4-), 101.02345 (C4H5O3-), 113.02363 (C5H5O3-), 119.03423 (C4H7O4-), 140.01122 (C2H7NPO4-), 152.99542 (C3H6PO5-), 376.10193 (C11H23NPO11-)	620.28357	286.21637 (C19H28NO+)
GPE		7.00	408.21609	78.95779 (PO3-), 96.96850 (H2PO4-), 152.99539 (C3H6PO5-), 171.00613 (C3H8PO6-), 334.17902 (C15H29NPO5-)	410.23059	98.06040 (C5H8NO+), 238.21635 (C15H28NO+)
GPE		7.01	420.21622	78.95781 (PO3-), 96.96849 (H2PO4-), 152.99533 (C3H6PO5-), 171.00604 (C3H8PO6-)	422.23072	250.21634 (C16H28NO+)
GPE		7.04	**596.28479**	59.01261 (C2H3O2-), 71.01265 (C3H3O2-), 78.95787 (PO3-), 89.02328 (C3H5O3-), 96.96852 (H2PO4-), 101.02336 (C4H5O3-), 113.02349 (C5H5O3-), 119.03413 (C4H7O4-), 152.99536 (C3H6PO5-), 333.05899 (C9H18PO11-)	598.29926	98.06040 (C5H8NO+), 264.23203 (C17H30NO+)
GPE		7.21	608.28406	59.01253 (C2H3O2-), 71.01255 (C3H3O2-), 78.95778 (PO3-), 89.02322 (C3H5O3-), 96.96848 (H2PO4-), 101.02331 (C4H5O3-), 113.02353 (C5H5O3-), 119.03403 (C4H7O4-), 152.99538 (C3H6PO5-), 333.05933 (C9H18PO11-)	610.29856	276.23196 (C18H30NO+)
EA		7.21	344.19998		310.23758	62.06079 (C2H8NO+), 292.22681 (C18H30NO2+)
GPE		7.22	452.24234	78.95779 (PO3-), 96.96850 (H2PO4-), 140.01120 (C2H7NPO4-), 152.99541 (C3H6PO5-), 171.00610 (C3H8PO6-), 214.04858 (C5H13NPO6-)	454.25684	86.06058 (C4H8NO+), 264.23193 (C17H30NO+), 282.24258 (C17H32NO2+)
GPE		7.24	**632.28479**	59.01255 (C2H3O2-), 71.01254 (C3H3O2-), 78.95777 (PO3-), 89.02318 (C3H5O3-), 96.96841 (H2PO4-), 101.02326 (C4H5O3-), 113.02338 (C5H5O3-), 119.03394 (C4H7O4-), 140.01123 (C2H7NPO4-), 152.99524 (C3H6PO5-), 171.00607 (C3H8PO6-), 196.03780 (C5H11NPO5-), 214.04849 (C5H13NPO6-),	634.29929	98.06040 (C5H8NO+), 124.07578 (C7H10NO+), 300.23190 (C20H30NO+)

				333.05911 (C9H18PO11-), 376.10114 (C11H23NPO11-)		
EA		7.29	334.21582		300.25333	62.06079 (C2H8NO+), 282.24252 (C17H32NO2+)
GPE		7.35	434.23141	78.95783 (PO3-), 96.96848 (H2PO4-), 152.99535 (C3H6PO5-), 171.00610 (C3H8PO6-), 2nd peak also has 140.01114 (C2H7NPO4-), 214.04854 (C5H13NPO6-)	436.24591	264.23203 (C17H30NO+)
GPE		7.37	410.23163	78.95777 (PO3-), 96.96846 (H2PO4-), 152.99533 (C3H6PO5-), 171.00606 (C3H8PO6-), 336.19443 (C15H31NPO5-)	412.24613	240.23204 (C15H30NO+)
GPE		7.38	**610.30048**	59.01254 (C2H3O2-), 71.01257 (C3H3O2-), 78.95781 (PO3-), 89.02328 (C3H5O3-), 96.96856 (H2PO4-), 101.02338 (C4H5O3-), 113.02358 (C5H5O3-), 119.03423 (C4H7O4-), 152.99541 (C3H6PO5-), 171.00616 (C3H8PO6-), 333.05923 (C9H18PO11-)	612.31458	278.24765 (C18H32ON+)
GPE		7.44	**598.30060**	59.01252 (C2H3O2-), 71.01255 (C3H3O2-), 78.95778 (PO3-), 89.02322 (C3H5O3-), 96.96844 (H2PO4-), 101.02332 (C4H5O3-), 113.02357 (C5H5O3-), 119.03406 (C4H7O4-), 152.99536 (C3H6PO5-), 171.00580 (C3H8PO6-), 333.05917 (C9H18PO11-)	600.31464	266.24762 (C17H32ON+)
GPE		7.57	446.23187	78.95776 (PO3-), 96.96846 (H2PO4-), 152.99536 (C3H6PO5-), 171.00606 (C3H8PO6-), 372.19406 (C18H31NPO5-)	448.24637	276.23199 (C18H30NO+)
GPE		7.59	822.36963	59.01249 (C2H3O2-), 71.01252 (C3H3O2-), 78.95777 (PO3-), 85.02821 (C4H5O2-), 89.02330 (C3H5O3-), 96.96840 (H2PO4-), 101.02325 (C4H5O3-), 113.02351 (C5H5O3-), 152.99548 (C3H6PO5-)	824.38413	184.07336 (C5H15NPO4+), 328.26343 (C22H34NO+)
		7.62	466.25781	1st peak has 59.01250 (C2H3O2-), 78.95769 (PO3-), 140.01103 (C2H7PO4-), 214.04845 (C5H13NPO6-), 269.21201 (C16H29O3-); 2nd peak has 78.95779 (PO3-), 96.96850 (H2PO4-), 140.01118 (C2H7PO4-), 152.99538 (C3H6PO5-), 171.00612 (C3H8PO6-), 214.04860 (C5H13NPO6-)		
GPE		7.63	470.23154	78.95778 (PO3-), 96.96850 (H2PO4-), 140.01118 (C2H7PO4-), 152.99538 (C3H6PO5-), 171.00612 (C3H8PO6-), 214.04858 (C5H13NPO6-)	472.24604	124.07578 (C7H10NO+), 300.23193 (C20H30NO+)
GPE		7.66	472.24744	78.95784 (PO3-), 96.96852 (H2PO4-), 152.99535 (C3H6PO5-), 171.00609 (C3H8PO6-), 2nd peak additionally has 140.01122 (C2H7PO4-), 214.04860 (C5H13NPO6-)	474.26194	302.24777 (C20H32NO+)
GPE		7.68	436.24716	78.95781 (PO3-), 96.96855 (H2PO4-), 152.99542 (C3H6PO5-), 171.00615 (C3H8PO6-), 362.20999 (C17H33NPO5-)	438.26175	266.24762 (C17H32ON+)
		7.79	424.24738		426.26188	254.24762 (C16H32NO+)
		7.88	724.27441			
GPE		8.25	474.26285	78.95782 (PO3-), 96.96849 (H2PO4-), 152.99532 (C3H6PO5-), 171.00606 (C3H8PO6-)	476.27735	304.26334 (C20H34NO+)
EA		9.75	372.23126		338.26868	62.06081 (C2H8NO+), 217.19504 (C16H25+), 259.20547 (C18H27O+), 320.25839 (C20H34NO2+)

EA		9.96	352.20535		318.24258	62.06080 (C2H8NO+), 300.23163 (C20H30NO+)
EA		10.25	330.22098		296.25842	62.06083 (C2H8NO+), 278.24796 (C18H32NO+), 279.23199 (C18H31O2+)
EA		10.63	354.22104		320.25833	62.06079 (C2H8NO+), 302.24847 (C20H32NO+)
EA		11.12	382.25238		348.28983	62.06082 (C2H8NO+), 330.27908 (C22H36NO+), 331.26379 (C22H35O2+, only 1st peak)

Table S4. Differential metabolites from *C. elegans* L1 medium, ES+ mode, that are decreased or absent in *daf-22* medium compared to N2. Peaks that are present but not differential in growth medium are shown in blue. Peaks that are also differential in growth medium are shown in red. **Peaks that are also in growth medium table (ES+) are shown in bold red.** Entries that have a corresponding peak in the ES- table are shaded grey.

class	*smid-db*	*rt (min)*	*m/z (ES+)*	*MS/MS (ES+)*	*m/z (ES-)*	*MS/MS (ES-)*
ascr		0.94	347.25381	72.08144 (C4H10N+), 84.08134 (C5H10N+), 101.10774 (C5H13N2+), 217.19107 (C11H25N2O2+)		
		0.95	375.26035	70.06583 (C4H8N+), 112.08727 (C5H10N3+), 118.08649 (C5H12NO2+), 210.16002 (C11H20N3O+), 228.17076 (C11H22N3O2+), 358.23364 (C17H32N3O5+)		
		0.96	404.31207	70.06592 (C4H8N+), 72.08149 (C4H10N+), 84.08131 (C5H10N+), 112.11236 (C7H14N+), 129.13867 (C7H17N2+)		
ascr		1.11	373.26987	84.08133 (C5H10N+), 127.12309 (C7H15N2+), 355.25900 (C19H35N2O4+)		
ascr		1.42	334.18622	see L1s, ES- table		
ascr	bhas#9	1.47	287.11014	see L1s, ES- table		
ascr		2.89	285.13120			
		2.89	308.20715	115.07573 (C6H11O2+)		
ascr		3.00	**316.21219**	55.05509 (C4H7+), 70.06583 (C4H8N+), 99.08086 (C6H11O+), 126.09148 (C7H12NO+), 186.14891 (C10H20NO2+), 200.12817 (C10H18NO3+)		
ascr		3.16	389.26471	84.08133 (C5H10N+), 114.09160 (C6H12NO+), 143.11794 (C7H15N2O+), 241.19069 (C13H25N2O2+), 259.20148 (C13H27N2O3+), 273.18069 (C13H25N2O4+)		
ascr		3.25	447.27020	72.08138 (C4H10N+), 86.09697 (C5H12N+), 98.09681 (C6H12N+), 100.07607 (C5H10NO+), 114.09164 (C6H12NO+), 157.13361 (C8H17N2O+), 201.12344 (C9H17N2O3+), 317.20676 (C15H29N2O5+)		
		3.27	383.22900			
ascr		3.27	369.23856	123.09186 (C7H11N2+), 239.17532 (C13H23N2O2+)		
ascr		3.29	374.25378	84.08135 (C5H10N+), 128.10713 (C7H14NO+)		
ascr		3.34	388.23294	100.07612 (C5H10NO+), 142.08636 (C7H12NO2+), 258.16998 (C13H24NO4+)		
S		3.39	306.10068	see L1s, ES- table		
ascr		3.39	461.28604	114.09165 (C6H12NO+), 138.09137 (C8H12NO+), 155.11789 (C8H15N2O+), 169.13345 (C9H17N2O+), 197.12852 (C10H17N2O2+), 215.13913 (C10H19N2O3+), 231.17030 (C11H23N2O3+), 331.22275 (C16H31N2O5+)		
ascr		3.49	**330.22763**	84.08132 (C5H10N+), 200.16452 (C11H22NO2+), 214.14372 (C11H20NO3+)		
EA		3.56	216.12321	62.06084 (C2H8NO+), 81.07048 (C6H9+), 109.06518 (C7H9O+), 127.07554 (C7H11O2+), 137.05978 (C8H9O2+), 170.11757 (C9H16NO2+), 180.10194 (C10H14NO2+), 198.11259 (C10H16NO3+)	214.10848	86.02355 (C3H4NO2-), 170.11836 (C9H16NO2-)
ascr		3.60	255.12036			
ascr		3.62	475.30209	114.09162 (C6H12NO+), 152.10703 (C9H14NO+), 169.13338 (C9H17N2O+), 213.12335 (C10H17N2O3+), 229.15469 (C11H21N2O3+), 345.23862 (C17H33N2O5+)		
ascr		3.78	318.22772	72.08147 (C4H10N+), 99.08088 (C6H11O+), 170.15393 (C10H20NO+), 184.13326 (C10H18NO2+), 188.16463 (C10H22NO2+), 202.14383 (C10H20NO3+)		
ascr	osas#14	3.80	681.26385	see L1s, ES- table		
		3.89	293.12323			
ascr		3.89	390.24841	99.08088 (C6H11O+), 116.10731		

				(C6H14NO+), 144.10197 (C7H14NO2+)		
ascr	osas#15	3.92	569.27057	see L1s, ES- table		
S		3.99	320.11633	84.04494 (C4H6NO+), 102.05531 (C4H8NO2+), 144.06554 (C6H10NO3+)	318.10168	66.03363 (C4H4N-), 110.02380 (C5H4NO2-), 142.05031 (C6H8NO3-), 175.04321 (C7H11SO3-)
ascr		3.99	333.12207	173.04849 (C6H13CaO3+), 191.05907 (C6H15CaO4+), 203.05910 (C7H15CaO4+), 217.07474 (C8H17CaO4+)		
ascr		4.09	331.10614	56.96560 (CaOH+), 173.4852 (C6H13CaO3+), 191.05902 (C6H15CaO4+), 201.04338 (C7H13CaO4+), 215.05904 (C8H15CaO4+)		
ascr	osas#16	4.26	549.24268	see L1s, ES- table		
ascr	glosas#9	4.31	510.19763	see 528.20850, 510.19763 in L1s, ES- table		
ascr	osas#23	4.41	565.31244	136.07578 (C8H10NO+), 200.16461 (C11H22NO2+), 218.08139 (C12H12NO3+), 236.09175 (C12H14NO4+), 348.14426 (C18H22NO6+)		
ascr		4.43	376.23325	see L1s, ES- table		
ascr	osas#24	4.63	550.22723	276.08438 (C12H15NO5Na+), 388.13629 (C18H23NO7Na+)	526.23096	59.01253 (C2H3O2-), 73.02815 (C3H5O3-), 82.02860 (C4H4NO-), 98.02366 (C4H4NO2-), 119.04939 (C8H7O-), 121.02865 (C7H5O2-), 133.0878 (C8H5O2-), 216.06671 (C12H10NO3-), 291.14514 (C13H23O7-, bhas#1)
ascr	glosas#2	4.69	661.31915	see L1s, ES- table		
ascr		4.78	303.09720	55.05509 (C4H7+), 76.97947 (C2H2OCl+), 83.04971 (C5H7O+), 85.06534 (C5H9O+), 113.06000 (C6H9O2+), 130.08633 (C6H12NO2+), 131.07037 (C6H11O3+), 133.04152 (C6H10OCl+), 148.09677 (C6H14NO3+), 151.05205 (C6H12O2Cl+),		
		4.88	450.23343	see L1s, ES- table		
ascr	ascr#81	4.93	393.16550	see L1s, ES- table		
		5.10	286.01563			
		5.20	297.16769	55.05507 (C4H7+), 109.10149 (C8H13+), 113.05997 (C6H9O2+), 127.11182 (C8H15O+), 130.08629 (C6H12NO2+), 131.07030 (C6H11O3+), 145.12228 (C8H17O2+), 148.09677 (C6H14NO3+)		
EA		5.29	258.17038	62.06081 (C2H8NO+), 107.08591 (C8H11+), 133.10126 (C10H13+), 151.11179 (C10H15O+), 179.10666 (C11H15O2+), 222.14883 (C13H20NO2+), 240.15942 (C13H22NO3+)		
		5.31	414.22516			
ascr		5.38	470.23608	104.10743 (C5H14NO+), 184.07335 (C10H11NONa+), 242.09966 (C9H17NO5Na+), 251.12526 (C12H20O4Na+), 340.17209 (C15H27NO6Na+)		
		5.40	553.25049	137.04582 (C5H5N4O+), 287.14923 (C14H23O6+)	551.23599	
ascr		5.46	492.22351			
ascr	osas#7	5.49	532.21613	see L1s, ES- table		
ascr	osas#25	5.56	494.23929	136.07574 (C8H10NO+), 200.07071 (C12H10NO2+), 218.08127 (C12H12NO3+), 236.09171 (C12H14NO4+), 348.14423 (C18H22NO6+)		
ascr	osas#1	5.56	534.23187	see L1s, ES- table		
S		5.62	374.16348	see L1s, ES- table		
ascr	osas#26	5.64	332.14948	101.02374 (C4H5O3+), 103.05470 (C8H7+), 113.06013 (C6H9O2+), 174.09152 (C11H12NO+), 184.07465 (C12H10NO+), 202.08632 (C12H12NO2+), 220.09694 (C12H14NO3+)		
ascr	nuclas#33, 34	5.73	697.30518	see L1s, ES- table		

		5.75	254.21161			
GPE		5.79	428.24146	see L1s, ES- table		
ascr	osas#22	5.87	498.18970	see L1s, ES- table		
ascr		5.91	528.20850	see 528.20850, 510.19763 in L1s, ES- table		
ascr	glosas#10, glosas#101	5.92	702.33417	see 528.20850, 510.19763 in L1s, ES- table		
S		6.04	345.14813	see L1s, ES- table		
		6.21	442.25711			
		6.22	488.22632	160.07321 (C8H11NONa+), 167.06798 (C7H12O3Na+), 251.12563 (C12H20O4Na+), 260.08902 (C12H15NO4Na+)		
ascr		6.41	325.19867	55.05507 (C4H7+), 81.07046 (C6H9+), 95.08597 (C7H11+), 113.06001 (C6H9O2+), 130.08638 (C6H12NO2+), 131.07031 (C6H11O3+), 137.13248 (C10H17+), 148.09676 (C6H14NO3+), 155.14301 (C10H19O+), 173.15358 (C10H21O2+)		
GPE		7.86	**634.29944**	see L1s, ES- table		
GPE		8.04	450.26187	see L1s, ES- table		
GPE		8.09	**600.31494**	see L1s, ES- table		
		14.77	605.33514			

Table S5. Differential metabolites from *C. elegans* growth medium, ES+ mode, that are decreased or absent in *daf-22* medium compared to N2. Peaks that are present but not differential in L1 medium are shown in blue. Peaks that are also differential in L1 medium are shown in red. **Peaks that are also in L1 medium table (ES+) are shown in bold red.** Manually added entries are shaded pink. Entries that have a corresponding peak in the ES- table are shaded grey.

class	*smid-db*	*rt (min)*	*m/z (ES+)*	*MS/MS (ES+)*	*m/z (ES-)*	*MS/MS (ES-)*
		0.96	268.20160			
ascr	uglas#11	2.87	669.20178	see growth medium, ES- table		
ascr		3.02	**316.21194**	see L1, ES+ table		
ascr		3.58	**330.22763**	see L1, ES+ table		
ascr		4.42	788.24023		786.22573	78.95783 (PO3-), 92.04945 (C6H6N-), 96.96856 (H2PO4-), 124.01461 (C4H2N3O2-), 136.03973 (C7H6NO2-), 150.03056 (C6H4N3O2-), 167.02078 (C5H3N4O3-), 178.02574 (C7H4N3O3-)
ascr		4.45	621.18109	see growth medium, ES- table		
ascr		4.64	211.03685	see growth medium, ES- table		
ascr	ascr#82	4.76	652.27191	see growth medium, ES- table		
ascr		4.96	640.24683	see growth medium, ES- table		
ascr		5.00	482.26001	see growth medium, ES- table		
ascr		5.05	794.28632	see growth medium, ES- table		
		5.13	373.12213			
ascr		5.17	576.18439	see growth medium, ES- table		
ascr	nuclas#35, 36	5.25	668.27832	see growth medium, ES- table		
		5.46	941.35510	136.06175 (C5H6N5+), 292.11786 (C15H18NO5+), 422.20306 (C19H28N5O6+), 427.17346, 525.14929	939.34060	78.95783 (PO3-), 96.96856 (H2PO4-)
		5.51	309.16736		285.17096	57.03328 (C3H5O-), 73.02824 (C3H5O2-), 87.04402 (C4H7O2-), 101.05977 (C5H9O2-), 115.07568 (C6H11O2-), 125.09643 (C8H13O-), 169.12325 (C10H17O2-), 241.18098 (C14H25O3-)
ascr		5.66	569.27179	109.06510 (C7H9O+), 127.07547 (C7H11O2+), 134.06007 (C8H8NO+), 213.12360 (C10H17N2O3+), 264.12317 (C14H18NO4+), 289.12857 (C13H31O7+)		
EA		5.68	232.19093	62.06082 (C2H8NO+), 214.18016 (C12H24NO2+)	266.15311	
ascr	anglas#7	5.71	556.23993	see growth medium, ES- table		
ascr	iglas#71	5.74	616.21661	see growth medium, ES- table		
EA		5.76	238.18028	62.06084 (C2H8NO+), 177.12737 (C12H17O+)		
ascr	iglas#9	5.78	527.26056			
ascr	anglas#1	5.79	558.25586	see growth medium, ES- table		
ascr	iglas#11	5.81	618.23218	see growth medium, ES- table		
		6.01	541.27655	115.07555 (C6H11O2+), 118.06532 (C8H8N+), 130.06516 (C9H8N+), 230.11736 (C14H16NO2+)		
ascr	nuclas#31, 32	6.11	580.29858	164.09306 (C7H10N5+), 450.23474 (C21H32N5O6+)		
ascr	iglas#7	6.20	536.25000	see growth medium, ES- table		
EA		6.21	246.20634	62.06082 (C2H8NO+), 228.19574 (C13H26NO2+)	280.16852	
ascr		6.32	644.24701	see growth medium, ES- table		
ascr	iglas#1	6.33	538.26520	see growth medium, ES- table		
		6.37	419.14505	see growth medium, ES- table		
ascr	anglas#3	6.39	584.27100	95.04955 (C6H7O+), 109.10147 (C8H13+), 113.05993 (C6H9O2+), 120.04453 (C7H6NO+), 127.03904 (C6H7O3+), 138.05490 (C7H8NO2+),	618.23328	

				155.10651 (C9H15O2+), 173.11714 (C9H17O3+), 228.06528 (C13H10NO3+), 250.10718 (C13H16NO4+), 263.12766 (C15H19O4+), 268.11780 (C13H18NO5+), 281.13806 (C15H21O5+), 299.14890 (C15H23O6+), 317.15912 (C15H25O7+), 400.17484 (C22H26NO6+), 418.18643 (C22H28NO7+), 436.19629 (C22H30NO8+)		
EA		6.67	284.22232	62.06081 (C2H8NO+), 266.21130 (C16H28NO2+)	318.1845, 328.21347	210.14990 (C12H20NO2-)
GPE		6.70	572.28406	see growth medium, ES- table		
EA		6.75	352.24823	62.06080 (C2H8NO+), 316.22699 (C20H30NO2+), 334.23685 (C20H32NO3+)	396.23938	262.18118 (C16H24NO2-)
GPE		6.78	584.28400	see growth medium, ES- table		
		6.81	704.34064	127.03909 (C6H7O3+), 136.07561 (C8H10NO+), 141.09120 (C8H13O2+), 159.10146 (C8H15O3+), 285.13284 (C14H21O6+), 295.19016 (C17H27O4+)	702.32600	
EA		6.81	274.23782	62.06080 (C2H8NO+), 256.22687 (C15H30NO2+)	308.20000, 318.22888	
EA		6.82	258.20651	see growth medium, ES- table		
ascr	iglas#3	6.82	581.30725			
EA		6.83	272.22192	62.06082 (C2H8NO+), 254.21123 (C15H28NO2+)		
ascr		6.87	581.30774	see growth medium, ES- table		
GPE		6.87	608.28345	see growth medium, ES- table		
		6.97	408.20172	106.02904 (C6H4NO+), 113.05995 (C6H9O2+), 124.03940 (C6H6NO2+), 178.08611 (C10H12NO2+), 236.09152 (C12H14NO4+), 254.10194 (C12H16NO5+)	406.18722	
EA		7.03	260.22202	see growth medium, ES- table		
EA		7.06	324.21695	62.06083 (C2H8NO+), 288.19537 (C18H26NO2+), 306.20636 (C18H28NO3+)	358.17913	
EA		7.07	598.29926	see growth medium, ES- table		
ascr	puglas#7	7.08	668.29645	134.04620 (C5H4N5+), 165.02325 (C6H5N4S+), 182.04944 (C6H8N5S+), 194.04953 (C7H8N5S+), 250.11186 (C11H16N5S+), 538.23254 (C24H36N5SO7+)		
ascr	puglas#1	7.16	670.31238	134.04613 (C5H4N5+), 152.05659 (C5H6N5O+), 165.02287 (C6H5N4S+), 182.04953 (C6H8N5S+), 194.04953 (C7H8N5S+), 224.05968 (C8H10N5SO+), 250.11194 (C11H16N5S+), 380.17499 (C17H26N5SO3+), 472.18652 (C19H30N5SO7+), 540.24896 (C24H38N5SO7+)		
GPE		7.21	620.28357	see growth medium, ES- table		
GPE		7.29	**634.29919**	see growth medium, ES- table		
EA		7.33	310.23758	see growth medium, ES- table		
EA		7.39	292.22702	62.06083 (C2H8NO+)		
EA		7.41	268.22708	62.06083 (C2H8NO+)		
GPE		7.45	438.26175	see growth medium, ES- table		
GPE		7.45	**600.31464**	see growth medium, ES- table		
	puglas#3	7.60	696.32758			
GPE		7.90	612.31458	see growth medium, ES- table		
EA		8.26	336.25296	62.06081 (C2H8NO+)	370.21514, 380.24457	
		8.26	266.24777			
EA		9.21	256.22696	62.06081 (C2H8NO+), 238.21642 (C15H28NO+), 239.20039 (C15H27O2+)	290.18914	
EA		9.26	244.22708	62.06081 (C2H8NO+), 226.21649 (C14H28NO+), 227.20047 (C14H27O2+)	278.18926	
		9.35	443.34775	112.07600 (C6H10NO+), 130.08635 (C6H12NO2+), 140.07057 (C7H10NO2+), 158.08115 (C7H12NO3+), 250.25275 (C17H32N+), 346.27353 (C22H36NO2+), 425.33777 (C24H45N2O4+)	477.30993	
EA		9.64	282.24268	62.06081 (C2H8NO+), 264.23169 (C17H30NO+), 265.21585 (C17H29O2+)	316.20486	
EA		9.65	314.26880	62.06082 (C2H8NO+), 296.25833	348.23098,	100.03935 (C4H6NO2-),

				(C18H34NO2+)	358.26010	102.05502 (C4H8NO2-)
EA		9.73	338.26868	see growth medium, ES- table		
EA		9.77	270.24255	62.06081 (C2H8NO+), 252.23170 (C16H30NO+), 253.21591 (C16H29O2+)	304.20473	
EA		9.86	258.24274	62.06079 (C2H8NO+), 240.23184 (C15H30NO+), 241.21596 (C15H29O2+)	292.20492, 302.23392	
EA		9.90	294.24265	62.06081 (C2H8NO+), 276.23203 (C18H30NO+), 277.21661 (C18H29O2+)	328.20483, 338.23401	
EA		9.92	318.24258	see growth medium, ES- table		
		10.07	586.42365	98.98460 (H4PO4+), 140.01082 (C2H7NPO4+), 155.04677 (C4H12PO4+), 211.10945 (C8H20PO4+), 267.17200 (C12H28PO4+), 320.25824 (C20H34NO2+)		
EA		10.11	320.25833	see growth medium, ES- table		
EA		10.18	308.25827	62.06081 (C2H8NO+), 290.24777 (C19H32NO+), 291.23239 (C19H31O2+)	342.22045	
EA		10.20	296.25842	see growth medium, ES- table		
EA		10.38	284.25839	62.06083 (C2H8NO+), 266.24774 (C17H32NO+), 267.23151 (C17H31O2+)	318.22057, 328.24960	
EA		10.61	272.25845	62.06081 (C2H8NO+), 254.24777 (C16H32NO+), 255.23174 (C16H31O2+)	306.22063, 316.24966	
EA		10.67	346.27405	62.06081 (C2H8NO+), 328.26282 (C22H34NO+)	380.23623, 390.26520	
EA		10.80	322.27420	62.06079 (C2H8NO+), 304.26352 (C20H34NO+)	356.23638, 366.26501	
EA		10.97	298.27399	62.06082 (C2H8NO+), 280.26331 (C18H34NO+), 281.24756 (C18H33O2+)	332.23617, 342.26517	
EA		11.08	348.28983	see growth medium, ES- table		
EA		11.75	350.30542	62.06083 (C2H8NO+), *332.29437 (C22H38NO+), *333.27859 (C22H37O2+); *only in the 2nd peak	384.2676, 394.29666	
EA		12.15	326.30548	62.06079 (C2H8NO+), 308.29468 (C20H38NO+), 309.27850 (C20H37O2+)	360.26766	

Table S6. Differential metabolites from *C. elegans* L1 medium, ES- mode, that are decreased or absent in N2 medium compared to *daf-22*. Peaks that are also differential in growth medium are shown in red. **Peaks that are also in growth medium table (ES-) are shown in bold red.** Entries that have a corresponding peak in the ES+ table are shaded grey.

class	*rt (min)*	*m/z (ES-)*	*MS/MS (ES-)*	*m/z (ES+)*	*MS/MS (ES+)*
GPE	1.13	486.03470	78.95782 (PO3-), 96.96855 (H2PO4-), 152.99547 (C3H6PO5-), 333.05939 (C9H18PO11-)	488.04901	153.98210 (C4H6NOCl2+)
GPE	1.18	323.98166	78.95779 (PO3-), 96.96844 (H2PO4-), 152.99535 (C3H6PO5-), 171.00615 (C3H8PO6-)	325.99576	82.94549 (CHCl2+), 153.98201 (C4H6NOCl2+)
	4.40	245.10333			
	4.92	391.19809	59.01260 (C2H3O2-), 71.01263 (C3H3O2-), 73.02826 (C3H5O2-), 83.01274 (C4H3O2-), 85.02834 (C4H5O2-), 101.02338 (C4H5O3-), 113.02346 (C5H5O3-)	410.23889, 415.19431	
GPE	5.07	498.24835	78.95783 (PO3-), 140.01138 (C2H7NPO4-), 152.99551 (C3H6PO5-), 171.00623 (C3H8PO6-), 214.04877 (C5H13NPO6-)		
GPE	5.29	**382.16431**	78.95782 (PO3-), 140.01129 (C2H7NPO4-), 152.99548 (C3H6PO5-), 171.00624 (C3H8PO6-), 214.04874 (C5H13NPO6-)	384.17881	
GPE	5.39	512.22736	first two peaks: 78.95784 (PO3-), 140.01129 (C2H7NPO4-), 152.99556 (C3H6PO5-), 171.00635 (C3H8PO6-), 214.04875 (C5H13NPO6-); 3rd peak: 78.95783 (PO3-), 96.96858 (H2PO4-), 152.99564 (C3H6PO5-), 350.17380 (C15H29NPO6-)		
GPE	5.61	538.24310	78.95785 (PO3-), 140.01137 (C2H7NPO4-), 152.99565 (C3H6PO5-), 171.00627 (C3H8PO6-), 214.04880 (C5H13NPO6-)	540.25760	
GPE	5.67	524.26355	78.95784 (PO3-), 140.01129 (C2H7NPO4-), 152.99547 (C3H6PO5-), 171.00612 (C3H8PO6-), 214.04872 (C5H13NPO6-)	526.27805	
GPE	5.68	512.26349	78.95783 (PO3-), 140.01129 (C2H7NPO4-), 152.99551 (C3H6PO5-), 171.00626 (C3H8PO6-), 214.04872 (C5H13NPO6-)	514.27799	
	5.72	395.18448		378.24869	181.15862 (C12H21O+), 199.16928 (C12H23O2+)
GPE	5.82	470.25281	78.95786 (PO3-), 96.96865 (H2PO4-), 152.99556 (C3H6PO5-), 171.00627 (C3H8PO6-), 214.04848 (C5H13NPO6-)	472.26731	
GPE	5.93	468.23712	78.95786 (PO3-), 140.01120 (C2H7NPO4-), 152.99544 (C3H6PO5-), 171.00616 (C3H8PO6-), 214.04865 (C5H13NPO6-)	452.24112, 470.25140, 492.23392	86.06057 (C4H8NO+), 280.22711 (C17H30NO2+)
EA	6.06	374.25534	100.03941 (C4H6NO2-), 102.05493 (C4H8NO2-), 271.19156 (C15H27O4-)	376.26947	62.06083 (C2H8NO+), 304.22687 (C19H30NO2+), 322.23764 (C19H32NO3+), 340.24820 (C19H34NO4+), 358.25821 (C19H36NO5+)
	6.22	429.14563		412.20975	
GPE	6.24	456.23746	78.95790 (PO3-), 96.96864 (H2PO4-), 140.01161 (C2H7NPO4-), 152.99562 (C3H6PO5-), 171.00627 (C3H8PO6-), 214.04898 (C5H13NPO6-)	458.25196	
S	6.67	384.18564	63.96117 (SO2-), 73.98193 (C2H2SO-), 84.04429 (C4H6NO-), 99.98524 (C3H2NSO-), 115.00887 (C4H5NSO-), 177.01006 (C5H7NSO4-)	386.19925	74.00652 (C2H4NS+), 116.01665 (C4H6NSO+), 120.01156 (C3H6NSO2+), 120.99554 (C3H5SO3+), 138.02193 (C3H8NSO3+), 162.02185 (C5H8NSO3+), 180.03246 (C5H10NSO4+), 189.16370 (C14H21+)
	7.27	287.22308		289.23758	
S	7.31	418.14670	63.96116 (SO2-), 99.98520 (C3H2NSO-), 115.00886 (C4H5NSO-), 177.01006 (C5H7NSO4-)	420.16120	
	7.33	**405.24982**	see growth medium, ES- table		
	7.37	**273.20749**	59.01257 (C2H3O2-)		
	7.63	295.19177	59.01252 (C2H3O2-), 87.04398 (C4H7O2-), 207.13919 (C13H19O2-)		
	7.67	489.34399	59.01259 (C2H3O2-), 73.02834 (C3H5O2-), 299.26010 (C18H35O3-)	491.35849, 513.34003	

	8.40	367.14517		369.15967	
GPE	8.49	642.32697	59.01258 (C2H3O2-), 71.01259 (C3H3O2-), 78.95784 (PO3-), 89.02328 (C3H5O3-), 96.96855 (H2PO4-), 101.02346 (C4H5O3-), 113.02355 (C5H5O3-), 119.03407 (C4H7O4-), 140.01123 (C2H7NPO4-), 152.99551 (C3H6PO5-), 171.00655 (C3H8PO6-), 333.05933 (C9H18PO11-), 376.10172 (C11H23NPO11-), 418.11206 (C13H25NPO12-), 480.27313 (C22H43NPO8-)	644.34147	86.06055 (C4H8NO+), 98.06044 (C5H8NO+), 292.26324 (C19H34NO+), 310.27386 (C19H36NO2+)
	8.51	517.37506	59.01260 (C2H3O2-)	519.38956, 541.37170	
	8.61	550.27118	78.95782 (PO3-), 275.20157 (C18H27O2-), 500.27737 (C25H43NPO7-)	516.30872	60.08154 (C3H10N+), 86.09695 (C5H12N+), 104.10734 (C5H14NO+), 124.99994 (C2H6PO4+), 184.07330 (C5H15NPO4+), 498.29874 (C26H45NPO6+)
	8.93	401.10605			
	8.94	323.22318	59.01258 (C2H3O2-)	325.23768, 347.21927	
	9.75	521.32538	73.02821 (C3H5O2-), 485.34872 (C27H49O7-)	509.34510	
GPE	10.37	770.24951	78.95789 (PO3-), 152.99547 (C3H6PO5-)	772.26401	
	11.26	454.35471	86.02370 (C3H4NO2-), 293.28476 (C20H37O-), 349.31137 (C23H41O2-), 367.32156 (C23H43O3-)	438.35837, 478.35092	MS/MS of 438.35837: 100.07610 (C5H10NO+), 420.34717 (C26H46NO3+); MS/MS of 478.35092: 337.27390 (C21H37O3+)
GPE	11.42	594.37872	78.95782 (PO3-), 96.96856 (H2PO4-), 140.01126 (C2H7NPO4-), 152.99547 (C3H6PO5-), 171.00621 (C3H8PO6-), 214.04869 (C5H13NPO6-)		
	11.68	**515.39594**	1st peak: 73.02826 (C3H5O2-), 367.32181 (C23H43O3-), 385.33298 (C23H45O4-); 2nd peak: 59.01257 (C2H3O2-), 73.02826 (C3H5O2-)	539.39234	
ascr	12.35	634.44684	71.01260 (C3H3O2-), 73.02824 (C3H5O2-), 83.04907 (C5H7O-), 86.02361 (C3H4NO2-), 111.04430 (C6H7O2-), 381.37433 (C25H49O2-), 511.43698 (C31H59O5-), 598.46948 (C34H64NO7-)	600.48389	62.06078 (C2H8NO+), 100.07603 (C5H10NO+), 434.39923 (C28H52NO2+), 452.40985 (C28H54NO3+)
ascr	12.69	**543.42737**	59.01258 (C2H3O2-), 73.02827 (C3H5O2-), 83.04922 (C5H7O-), 111.04433 (C6H7O2-)	567.42358	
ascr	13.18	533.36206	73.02825 (C3H5O2-), 83.04896 (C5H7O-), 111.04438 (C6H7O2-), 497.38492 (C29H53O6-)		
	13.28	668.40765		656.42676	
ascr	15.96	581.44305	59.01266 (C2H3O2-), 73.02834 (C3H5O2-), 83.04920 (C5H7O-), 111.04437 (C6H7O2-), 409.36954 (C26H49O3-), 521.42023 (C32H57O5-), 539.43195 (C32H59O6-)	605.43945	

Table S7. Differential metabolites from *C. elegans* growth medium, ES- mode, that are decreased or absent in N2 medium compared to *daf-22*. Peaks that are also differential in L1 medium are shown in red. **Peaks that are also in L1 medium table (ES-) are shown in bold red.** Entries that have a corresponding peak in the ES+ table are shaded grey.

class	*rt (min)*	*m/z (ES-)*	*MS/MS (ES-)*	*m/z (ES+)*	*MS/MS (ES+)*
	2.92	268.17816	111.01894 (C4H3N2O2-), 168.09033 (C6H10N5O-), 169. 08533, 186.13303 (C7H16N5O-), 226.15607 (C11H20N3O2-), 251.15167 (C12H19N4O2-)		
GPE	4.84	370.16397	78.95776 (PO3-), 96.96848 (H2PO4-), 152.99533 (C3H6PO5-), 171.00607 (C3H8PO6-), 214.04854 (C5H13NPO6-)	372.17847	
	4.93	296.12729	78.95776 (PO3-), 96.96847 (H2PO4-)	298.14179	
GPE	5.00	**382.16422**	see L1s, ES- table		
	5.03	294.11142	78.95778 (PO3-), 96.96848 (H2PO4-), 140.01118 (C2H7NPO4-)	296.12592	
	5.49	470.18018	78.95786 (PO3-), 96.96861 (H2PO4-), 140.01123 (C2H7NPO4-), 182.02219 (C4H9NPO5-), 259.02258 (C6H12PO9-), 302.06454 (C8H17NPO9-)	494.17658	
GPE	5.78	560.24799	59.01263 (C2H3O2-), 71.01256 (C3H3O2-), 78.95784 (PO3-), 89.02323 (C3H5O3-), 96.96851 (H2PO4-), 101.02345 (C4H5O3-), 113.02349 (C5H5O3-), 119.03407 (C4H7O4-), 140.01112 (C2H7NPO4-), 152.99536 (C3H6PO5-), 171.00615 (C3H8PO6-), 333.05908 (C9H18PO11-), 376.10165 (C11H23NPO11-)	562.26249	
	5.84	308.12741	78.95779 (PO3-), 96.96844 (H2PO4-), *140.01117 (C2H7NPO4-); (* only in 2nd peak)	310.14191	
	5.94	214.14528	57.03327 (C3H5O-), 86.02356 (C3H4NO2-), 127.11205 (C8H15O-)	216.15970	62.06083 (C2H8NO+), 86.06059 (C4H8NO+), 95.08598 (C7H11+), 198.14888 (C11H20NO2+)
GPE	5.97	618.29047	59.01257 (C2H3O2-), 71.01257 (C3H3O2-), 78.95780 (PO3-), 89.02326 (C3H5O3-), 96.96847 (H2PO4-), 101.02330 (C4H5O3-), 113.02340 (C5H5O3-), 152.99530 (C3H6PO5-), 333.05865 (C9H18PO11-)	620.30497	
	6.03	346.22397	100.03944 (C4H6NO2-), 102.05499 (C4H8NO2-)	302.23297	
GPE	6.16	616.27448	59.01264 (C2H3O2-), 71.01261 (C3H3O2-), 78.95786 (PO3-), 89.02328 (C3H5O3-), 101.02336 (C4H5O3-), 113.02328 (C5H5O3-), 119.03419 (C4H7O4-), 140.01122 (C2H7NPO4-), 152.99529 (C3H6PO5-), 196.03816 (C5H11NPO5-), 214.04877 (C5H13NPO6-), 376.10126 (C11H23NPO11-)	640.27088	
	6.17	303.21796	59.01253 (C2H3O2-), 243.19670 (C14H27O3-)	305.23246	
GPE	6.28	548.26367	78.95772 (PO3-), 140.01096 (C2H7NPO4-), 152.99518 (C3H6PO5-), 214.04852 (C5H13NPO6-)	550.27817	
	6.36	231.16019	59.01253 (C2H3O2-), 171.13873 (C10H19O2-)		
	6.40	433.19995	78.95779 (PO3-), 96.96851 (H2PO4-)	435.21460	301.21588 (C20H29O2+), 319.22668 (C20H31O3+)
GPE	6.47	670.32196	59.01255 (C2H3O2-), 71.01257 (C3H3O2-), 78.95781 (PO3-), 89.02323 (C3H5O3-), 96.96853 (H2PO4-), 101.02341 (C4H5O3-), 113.02347 (C5H5O3-), 119.03407 (C4H7O4-), 140.01128 (C2H7NPO4-), 152.99541 (C3H6PO5-), 171.00607 (C3H8PO6-), *196.03784 (C5H11NPO5-), 333.05951 (C9H18PO11-), 376.10147 (C11H23NPO11-); (* only in 2nd peak)	672.33612	86.06060 (C4H8NO+), *112.03963 (C5H6NO2+), 302.24774 (C20H32NO+), 320.25836 (C20H34NO2+), 338.26883 (C20H36NO3+); (* only in 7.2 min peak)
	6.50	315.21786	59.01255 (C2H3O2-), 255.19638 (C15H27O3-)	317.23236	
GPE	6.50	658.32166	59.01254 (C2H3O2-), 71.01254 (C3H3O2-), 78.95776 (PO3-), 89.02318 (C3H5O3-), 101.02325 (C4H5O3-), 113.02338 (C5H5O3-), 119.03397 (C4H7O4-), 140.01102 (C2H7NPO4-), 152.99515 (C3H6PO5-), 196.03784 (C5H11NPO5-), 214.04881 (C5H13NPO6-), 333.05975 (C9H18PO11-), 376.10114 (C11H23NPO11-)	660.33594	86.06059 (C4H8NO+), 308.25827 (C19H34NO2+), 326.26880 (C19H36NO3+)
	6.51	243.16025	59.01256 (C2H3O2-)		
EA	6.53	362.25516	100.03936 (C4H6NO2-), 102.05502 (C4H8NO2-)	318.26416	62.06081 (C2H8NO+), 282.24252 (C17H32NO2+), 300.25311 (C17H34NO3+)
	6.54	317.19717	59.01258 (C2H3O2-), 129.05504 (C6H9O3-),	341.19357	

			195.17531 (C13H23O-), 255.19687 (C15H27O3-), 257.17551 (C14H25O4-), 299.18658 (C16H27O5-)		
EA	6.57	348.23935	100.03934 (C4H6NO2-), 102.05499 (C4H8NO2-), 199.17055 (C12H23O2-)	304.24826	62.06081 (C2H8NO+), 268.22687 (C16H30NO2+), 286.23743 (C16H32NO3+)
	6.63	515.28632	59.01253 (C2H3O2-), 71.01254 (C3H3O2-), 89.02335 (C3H5O3-), 101.02341 (C4H5O3-), 113.02348 (C5H5O3-)		
GPE	6.65	646.32141	59.01253 (C2H3O2-), 71.01257 (C3H3O2-), 78.95777 (PO3-), 89.02323 (C3H5O3-), 96.96848 (H2PO4-), 101.02336 (C4H5O3-), 113.02354 (C5H5O3-), 119.03410 (C4H7O4-), 140.01131 (C2H7NPO4-), 152.99536 (C3H6PO5-), 171.00624 (C3H8PO6-), 333.05911 (C9H18PO11-), 376.10126 (C11H23NPO11-)	648.33557	86.06059 (C4H8NO+), 278.24780 (C18H32NO+), 296.25845 (C18H34NO2+), 314.26892 (C18H36NO3+)
EA	6.70	526.27924	71.01247 (C3H3O2-), 101.02342 (C4H5O3-), 403.26962 (C21H39O7-)	492.31706	62.06083 (C2H8NO+), 86.06059 (C4H8NO+), 294.24261 (C18H32NO2+), 312.25314 (C18H34NO3+)
EA	6.78	370.26010		372.27460	6.3 and 6.75 min: 62.06082 (C2H8NO+), **251.20030 (C16H27O2+), *257.18979 (C18H25O+), 275.20044 (C18H27O2+), 293.21097 (C18H29O3+), **311.22168 (C18H31O4+), *318.24268 (C20H32NO2+), 336.25339 (C20H34NO3+), 354.26376 (C20H36NO4+); (* only in 1st peak, ** only in 2nd peak)
	6.78	314.23407	57.03325 (C3H5O-), 86.02354 (C3H4NO2-), 211.17027 (C13H23O2-), 227.20154 (C14H27O2-)	316.24857	62.06082 (C2H8NO+), 86.06059 (C4H8NO+), 280.22693 (C17H30NO2+), 298.23746 (C17H32NO3+)
	6.82	228.16058	57.03328 (C3H5O-), 86.02355 (C3H4NO2-), 141.12796 (C9H17O-)	230.17508	
GPE	6.85	672.33771	59.01252 (C2H3O2-), 71.01255 (C3H3O2-), 78.95777 (PO3-), 89.02321 (C3H5O3-), 96.96848 (H2PO4-), 101.02332 (C4H5O3-), 113.02347 (C5H5O3-), 119.03410 (C4H7O4-), 152.99535 (C3H6PO5-), 171.00618 (C3H8PO6-), 333.05930 (C9H18PO11-), 376.10138 (C11H23NPO11-)	674.35205	86.06059 (C4H8NO+), 304.26318 (C20H34NO+), 322.27374 (C20H36NO2+), 340.28430 (C20H38NO3+)
	6.86	473.27591	59.01255 (C2H3O2-), 71.01258 (C3H3O2-), 89.02328 (C3H5O3-), 101.02336 (C4H5O3-), 113.02352 (C5H5O3-), 119.03411 (C4H7O4-), 455.26495 (C24H39O8-)	492.31696	217.19505 (C16H25+), 235.20549 (C16H27O+), 241.19482 (C18H25+), 259.20529 (C18H27O+), 277.21613 (C18H29O2+), 295.22665 (C18H31O3+)
EA	6.90	442.28156		398.29037	62.06081 (C2H8NO+), 84.08134 (C5H10N+), 344.25851 (C22H34NO2+), 362.26846 (C22H36NO3+), 380.27863 (C22H38NO4+)
	6.93	245.17601	59.01255 (C2H3O2-), 185.15448 (C11H21O2-)		
	6.94	461.27594			
GPE	6.96	666.29034	59.01223 (C2H3O2-), 71.01229 (C3H3O2-), 78.95791 (PO3-), 89.02337 (C3H5O3-), 101.02343 (C4H5O3-), 113.02356 (C5H5O3-), 119.03415 (C4H7O4-), 140.01120 (C2H7NPO4-), 152.99541 (C3H6PO5-), 196.03781 (C5H11NPO5-), 333.05957 (C9H18PO11-), 376.10117 (C11H23NPO11-)	690.28674	
	7.03	619.33392	59.01261 (C2H3O2-), 71.01260 (C3H3O2-), 89.02325 (C3H5O3-), 101.02331 (C4H5O3-), 113.02349 (C5H5O3-), 119.03407 (C4H7O4-), 131.03424 (C5H7O4-), 161.04501 (C6H9O5-), 221.06644 (C8H13O7-), 277.21686 (C18H29O2-)	638.37524	85.02894 (C4H5O2+), 97.02877 (C5H5O2+), 127.03906 (C6H7O3+), 145.04956 (C6H9O4+), 261.22104 (C18H29O+), 279.23160 (C18H31O2+)
	7.10	391.18982	78.95779 (PO3-), 96.96850 (H2PO4-)	393.20432	
EA	7.11	394.26016	57.03328 (C3H5O-), 86.02367 (C3H4NO2-), 87.04408 (C4H7O2-), 219.17548 (C15H23O-), 254.17548 (C17H20NO-), 307.22791 (C19H31O3-)	396.27466	62.06082 (C2H8NO+), 275.20020 (C18H27O2+), 299.19980 (C20H27O2+), 317.21088 (C20H29O3+), 342.24222 (C22H32O2N+), 360.25278

					(C22H34O3N+), 378.26349 (C22H36O4N+)
	7.16	419.26566	59.01254 (C2H3O2-), 71.01256 (C3H3O2-), 101.02329 (C4H5O3-), 257.21219 (C15H29O3-)		
GPE	7.19	510.28391	78.95777 (PO3-), 96.96841 (H2PO4-), 140.01109 (C2H7NPO4-), 152.99530 (C3H6PO5-), 171.00603 (C3H8PO6-), 214.04860 (C5H13NPO6-)		
	7.19	387.19470	78.95778 (PO3-), 96.96848 (H2PO4-)	389.20892	
GPE	7.22	754.42700	59.01253 (C2H3O2-), 71.01257 (C3H3O2-), 78.95778 (PO3-), 89.02324 (C3H5O3-), 101.02337 (C4H5O3-), 113.02341 (C5H5O3-), 119.03418 (C4H7O4-), 140.01117 (C2H7NPO4-), 152.99533 (C3H6PO5-), 196.03793 (C5H11NPO5-), 214.04855 (C5H13NPO6-), 333.05994 (C9H18PO11-), 376.10132 (C11H23NPO11-), 640.31067 (C28H51O13NP-), 652.31146 (C29H51O13NP-)	756.44116	84.08132 (C5H10N+), 86.06059 (C4H8NO+), 98.09686 (C6H12N+), 115.12326 (C6H15N2+), 308.25830 (C19H34NO2+)
	7.23	475.29160	1st peak: 59.01258 (C2H3O2-), 71.01263 (C3H3O2-), 89.02335 (C3H5O3-), 101.02338 (C4H5O3-), 113.02358 (C5H5O3-), 119.03407 (C4H7O4-)	1st peak: 494.3321, 2nd peak: 448.32715	
	7.25	269.17609	59.01257 (C2H3O2-), 181.15936 (C12H21O-)		
	7.26	**405.24966**	59.01254 (C2H3O2-), 71.01256 (C3H3O2-), 85.02828 (C4H5O2-), 89.02320 (C3H5O3-), 101.02332 (C4H5O3-), 113.02348 (C5H5O3-), 119.03400 (C4H7O4-), 225.18605 (C14H25O2-), 243.19635 (C14H27O3-)		
	7.28	259.19156	59.01254 (C2H3O2-), 199.17014 (C12H23O2-)		
	7.31	**273.20740**	59.01263 (C2H3O2-)		
	7.31	309.17117	59.01253 (C2H3O2-), 247.17043 (C16H23O2-), 249.14906 (C15H21O3-)		
	7.32	592.27716	193.15950 (C13H21O-), 237.14934 (C14H21O3-)	548.28595	120.08095 (C8H10N+), 166.08618 (C9H12NO2+), 239.16400 (C14H23O3+), 292.11768 (C15H18NO5+), 310.12823 (C15H20NO6+), glucose fragments
	7.35	515.28656	59.01250 (C2H3O2-), 71.01253 (C3H3O2-), 85.02828 (C4H5O2-), 89.02324 (C3H5O3-), 101.02332 (C4H5O3-), 113.02367 (C5H5O3-), 119.03407 (C4H7O4-), 161.04514 (C6H9O5-)	488.32214, 493.27744	
	7.36	242.17653	57.03332 (C3H5O-), 86.02360 (C3H4NO2-), 155.14365 (C10H19O-)	244.19103	
	7.40	343.24927	59.01250 (C2H3O2-)	345.26377, 367.24548	
	7.41	419.26553	59.01254 (C2H3O2-), 71.01256 (C3H3O2-), 101.02329 (C4H5O3-), 257.21219 (C15H29O3-)		
GPE	7.42	668.30634	59.01256 (C2H3O2-), 71.01257 (C3H3O2-), 78.95779 (PO3-), 89.02322 (C3H5O3-), 101.02330 (C4H5O3-), 113.02344 (C5H5O3-), 119.03404 (C4H7O4-), 140.01111 (C2H7NPO4-), 152.99530 (C3H6PO5-), 196.03784 (C5H11NPO5-), 214.04851 (C5H13NPO6-), 333.05917 (C9H18PO11-), 376.10123 (C11H23NPO11-)		
	7.46	417.20520	78.95776 (PO3-), 96.96841 (H2PO4-)	419.21970	
	7.47	297.20740	1st peak: 155.10735 (C9H15O2-); 2nd peak: 59.01251 (C2H3O2-)	299.2219, 321.20358	
GPE	7.50	694.32153	59.01252 (C2H3O2-), 71.01254 (C3H3O2-), 78.95777 (PO3-), 89.02322 (C3H5O3-), 101.02332 (C4H5O3-), 113.02348 (C5H5O3-), 119.03411 (C4H7O4-), 140.01117 (C2H7NPO4-), 152.99538 (C3H6PO5-), 196.03781 (C5H11NPO5-), 214.04851 (C5H13NPO6-), 333.05875 (C9H18PO11-), 376.10120 (C11H23NPO11-)	696.33603	
GPE	7.54	600.27966	59.01254 (C2H3O2-), 71.01257 (C3H3O2-), 78.95781 (PO3-), 89.02324 (C3H5O3-), 101.02336 (C4H5O3-), 113.02357 (C5H5O3-), 119.03413 (C4H7O4-), 140.01123 (C2H7NPO4-), 152.99544 (C3H6PO5-), 196.03790 (C5H11NPO5-), 214.04868 (C5H13NPO6-), 333.05988 (C9H18PO11-), 376.10153 (C11H23NPO11-)	602.29416	
	7.54	400.27063	100.03931 (C4H6NO2-), 102.05501 (C4H8NO2-), 251.20146 (C16H27O2-)	356.27963	

	7.56	353.23358	59.01253 (C2H3O2-), 87.04396 (C4H7O2-), 335.22235 (C20H31O4-)	355.24808	
	7.57	393.20572	78.95787 (PO3-), 96.96854 (H2PO4-)	395.22022	
GPE	7.60	674.35291	59.01252 (C2H3O2-), 71.01257 (C3H3O2-), 78.95777 (PO3-), 89.02325 (C3H5O3-), 96.96851 (H2PO4-), 101.02333 (C4H5O3-), 119.03416 (C4H7O4-), 140.01115 (C2H7NPO4-), 152.99536 (C3H6PO5-), 333.05978 (C9H18PO11-), 376.10102 (C11H23NPO11-)	676.36749	86.06059 (C4H8NO+), 306.27896 (C20H36NO+), 324.28955 (C20H38NO2+), 342.30011 (C20H40NO3+)
GPE	7.65	692.30615	59.01256 (C2H3O2-), 71.01264 (C3H3O2-), 78.95791 (PO3-), 89.02338 (C3H5O3-), 101.02345 (C4H5O3-), 113.02357 (C5H5O3-), 119.03415 (C4H7O4-), 140.01125 (C2H7NPO4-), 152.99554 (C3H6PO5-), 196.03778 (C5H11NPO5-), 214.04852 (C5H13NPO6-), 333.05911 (C9H18PO11-), 376.10123 (C11H23NPO11-)	694.32031	86.06058 (C4H8NO+), 112.03960 (C5H6NO2+), 128.07072 (C6H10NO2+), 342.24258 (C22H32NO2+), 360.25305 (C22H34NO3+)
	7.67	323.18674	59.01253 (C2H3O2-), 261.18588 (C17H25O2-), 263.16544 (C16H23O3-), 305.17603 (C18H25O4-)		
	7.67	491.19284	93.03342 (C6H5O-), 137.02379 (C7H5O3-), 141.12782 (C9H17O-), 165.12813 (C11H17O-), 167.10759 (C10H15O2-), 209.11823 (C12H17O3-), 281.06638 (C13H13O7-)	493.20734	
	7.70	271.19177	59.01253 (C2H3O2-), 209.19109 (C14H25O-)	273.20627	
	7.73	283.19180	59.01254 (C2H3O2-)	285.20630	
	7.77	299.22296	1st peak: 209.15468 (C13H21O2-), 239.20151 (C15H27O2-), 253.14435 (C14H21O4-); 2nd peak: 59.01254 (C2H3O2-), 237.22261 (C16H29O-)	301.23746	
	7.77	342.26526	57.03328 (C3H5O-), 86.02369 (C3H4NO2-), 239.20164 (C15H27O2-), 255.23297 (C16H31O2-)	344.27976, 366.26144	
	7.78	803.36066	59.01260 (C2H3O2-), 71.01263 (C3H3O2-), 78.95778 (PO3-), 89.02333 (C3H5O3-), 94.03996 (C4H4N3-), 96.96845 (H2PO4-), 101.02337 (C4H5O3-), 108.01938 (C4H2N3O-), 126.02992 (C4H4N3O2-), 133.01477 (C5HN4O), 150.04163 (C5H4N5O-), 152.99530 (C3H6PO5-), 171.00597 (C3H8PO6-), 333.05911 (C9H18PO11-), 358.25034 (C21H32N5O3-), 376.10226 (C11H23NPO11-), 426.25146 (C23H32N5O3-), 652.31055 (C29H51NPO13-)	805.37469	126.05506 (C6H8NO2+), 152.05669 (C5H6N5O+), 206.06717 (C8H8N5O2+), 320.25824 (C20H34NO2+), 471.30801 (C25H39N6O3+), 643.32178 (C28H48N6PO9+)
	7.79	461.27634	1st peak: 59.01257 (C2H3O2-), 71.01259 (C3H3O2-), 89.02322 (C3H5O3-), 101.02332 (C4H5O3-), 113.02344 (C5H5O3-)	434.31122, 439.26660 (only for 2nd peak)	
GPE	7.80	669.33759	59.01253 (C2H3O2-), 71.01255 (C3H3O2-), 78.95778 (PO3-), 89.02323 (C3H5O3-), 101.02335 (C4H5O3-), 113.02350 (C5H5O3-), 119.03408 (C4H7O4-), 140.01118 (C2H7NPO4-), 152.99538 (C3H6PO5-), 171.00626 (C3H8PO6-), 196.03799 (C5H11NPO5-), 214.04878 (C5H13NPO6-), 333.05917 (C9H18PO11-), 376.10123 (C11H23NPO11-)	671.35181	86.06055 (C4H8NO+), 112.03957 (C5H6NO2+), 308.25815 (C19H34NO2+), 480.27286 (C22H43NPO8+)
	7.83	357.26489	59.01253 (C2H3O2-)	359.27939, 381.26102	
GPE	7.83	787.36560	59.01265 (C2H3O2-), 71.01262 (C3H3O2-), 78.95787 (PO3-), 89.02326 (C3H5O3-), 96.96863 (H2PO4-), 101.02344 (C4H5O3-), 134.04654 (C5H4N5-), 152.99542 (C3H6PO5-), 333.05917 (C9H18PO11-), 652.31042 (C29H51NPO13-)	789.38010	
	7.84	457.28104	59.01253 (C2H3O2-), 71.01254 (C3H3O2-), 85.02827 (C4H5O2-), 89.02322 (C3H5O3-), 101.02334 (C4H5O3-), 113.02350 (C5H5O3-), 119.03418 (C4H7O4-), 277.21704 (C18H29O2-), 295.22778 (C18H31O3-)	459.29554, 476.32220	
	7.87	313.20230	59.01255 (C2H3O2-), 251.20143 (C16H27O2-), 253.18069 (C15H25O3-), 295.19089 (C17H27O4-)		
	7.90	352.24954	7.9 min: 57.03331 (C3H5O-), 86.02359 (C3H4NO2-), 111.08054 (C7H11O-), 153.12810 (C10H17O-); 8.2 min: 57.03329 (C3H5O-), 86.02367 (C3H4NO2-), 113.09635 (C7H13O-), 247.20657 (C17H27O-); 9.1 min: 86.02364 (C3H4NO2-), 115.07561 (C6H11O2-), 265.21722 (C17H29O2-)	354.26404	
GPE	7.91	723.38495	59.01251 (C2H3O2-), 71.01254 (C3H3O2-), 78.95776 (PO3-), 89.02320 (C3H5O3-), 101.02331 (C4H5O3-),		

			113.02348 (C5H5O3-), 119.03407 (C4H7O4-), 140.01112 (C2H7NPO4-), 152.99532 (C3H6PO5-), 196.03786 (C5H11NPO5-), 214.04851 (C5H13NPO6-), 333.05920 (C9H18PO11-), 376.10110 (C11H23NPO11-), 640.31067 (C28H51NPO13-)		
GPE	7.92	614.29523	59.01253 (C2H3O2-), 71.01253 (C3H3O2-), 78.95774 (PO3-), 89.02316 (C3H5O3-), 101.02322 (C4H5O3-), 113.02333 (C5H5O3-), 119.03391 (C4H7O4-), 140.01100 (C2H7NPO4-), 152.99525 (C3H6PO5-), 196.03790 (C5H11NPO5-), 214.04857 (C5H13NPO6-), 333.05917 (C9H18PO11-), 376.10123 (C11H23NPO11-)	616.30975	86.06059 (C4H8NO+), 282.24255 (C17H32NO2+)
	7.97	352.22650			
GPE	7.98	438.22638	78.95782 (PO3-), 140.01129 (C2H7NPO4-), 152.99542 (C3H6PO5-), 214.04861 (C5H13NPO6-)	440.24088	
EA	7.98	426.28662	100.03931 (C4H6NO2-), 102.05490 (C4H8NO2-)	382.29562	62.06081 (C2H8NO+), 346.27396 (C22H36NO2+), 364.28397 (C22H38NO3+)
	8.03	402.28641	100.03925 (C4H6NO2-), 102.05492 (C4H8NO2-), 139.11212 (C9H15O-), 253.21695 (C16H29O2-)	358.29541	
	8.07	374.25504	57.03329 (C3H5O-), 86.02356 (C3H4NO2-), 239.20163 (C15H27O2-), 241.21721 (C15H29O2-)	330.26404	
	8.10	376.27072	100.03934 (C4H6NO2-), 102.05497 (C4H8NO2-), 227.20148 (C14H27O2-)	332.27972	
	8.10	293.17630	59.01253 (C2H3O2-)	295.19080	
	8.18	319.19174	59.01253 (C2H3O2-)	321.20624	
	8.19	499.29193		472.32693	
	8.22	770.24408			
	8.23	378.26541	57.03327 (C3H5O-), 86.02357 (C3H4NO2-), 219.17531 (C15H23O-), 291.23340 (C19H31O2-)	380.27991	
	8.26	285.20740	59.01253 (C2H3O2-)	287.22190	
	8.28	758.24365			
	8.29	710.31390		644.34110	86.06059 (C4H8NO+), 98.06046 (C5H8NO+), 292.26334 (C19H34NO+), 310.27390 (C19H36NO2+)
	8.30	772.28497			
GPE	8.31	676.31061	59.01253 (C2H3O2-), 71.01255 (C3H3O2-), 78.95778 (PO3-), 89.02323 (C3H5O3-), 101.02338 (C4H5O3-), 113.02348 (C5H5O3-), 119.03409 (C4H7O4-), 140.01120 (C2H7NPO4-), 152.99539 (C3H6PO5-), 196.03787 (C5H11NPO5-), 214.04852 (C5H13NPO6-), 333.06006 (C9H18PO11-), 376.10141 (C11H23NPO11-)	678.32511	
	8.33	846.46222		848.47672	
GPE	8.34	652.31097	59.01252 (C2H3O2-), 71.01255 (C3H3O2-), 78.95778 (PO3-), 89.02321 (C3H5O3-), 101.02332 (C4H5O3-), 113.02348 (C5H5O3-), 119.03410 (C4H7O4-), 140.01117 (C2H7NPO4-), 152.99538 (C3H6PO5-), 196.03784 (C5H11NPO5-), 214.04849 (C5H13NPO6-), 333.05930 (C9H18PO11-), 376.10120 (C11H23NPO11-)	654.32550	diff. peak: 86.06059 (C4H8NO+), 320.25836 (C20H34NO2+); later peak: 100.07613 (C5H10NO+), 126.05511 (C6H8NO2+), 320.25836 (C20H34NO2+)
GPE	8.41	640.31073	59.01252 (C2H3O2-), 71.01254 (C3H3O2-), 78.95776 (PO3-), 89.02321 (C3H5O3-), 101.02331 (C4H5O3-), 113.02347 (C5H5O3-), 119.03407 (C4H7O4-), 140.01114 (C2H7NPO4-), 152.99535 (C3H6PO5-), 196.03780 (C5H11NPO5-), 214.04851 (C5H13NPO6-), 333.05923 (C9H18PO11-), 376.10117 (C11H23NPO11-)	642.32513	86.06061 (C4H8NO+), 308.25833 (C19H34NO2+)
	8.44	844.44678		846.46128	
	8.45	321.20718	59.01253 (C2H3O2-)	323.22168	
	8.46	354.26508	8.46 min: 57.03326 (C3H5O-), 86.02354 (C3H4NO2-), 113.09646 (C7H13O-), 153.12807 (C10H17O-), 267.23294 (C17H32O2-); 8.65 min: 57.03323 (C3H5O-), 86.02357 (C3H4NO2-), 141.09154 (C8H13O2-), 267.23279 (C17H32O2-); 9.65 min: 57.03330 (C3H5O-), 86.02353 (C3H4NO2-), 169.15958 (C11H21O-), 267.23267 (C17H32O2-)	356.27948	8.4 min: 62.06082 (C2H8NO+), 217.19510 (C16H25+), 259.20563 (C18H27O+), 320.25830 (C20H34NO2+), 338.26880 (C20H36NO3+); 9.7 min: 62.06083 (C2H8NO+), 217.19498 (C16H25+), 235.20555 (C16H27O+), 253.21631 (C16H29O2+), 271.22653 (C16H31O3+), 295.22662 (C18H31O3+), 338.26920

					(C20H36NO3+)
	8.46	431.30139	59.01253 (C2H3O2-)	450.34189	
	8.47	568.28955	78.95776 (PO3-), 96.96840 (H2PO4-), 406.23679 (C19H37NPO6-)		
GPE	8.48	452.24213	78.95779 (PO3-), 140.01117 (C2H7NPO4-), 152.99535 (C3H6PO5-), 171.00612 (C3H8PO6-), 214.04857 (C5H13NPO6-)	454.25663	
GPE	8.61	807.38458	78.95780 (PO3-), 86.02342 (C3H4NO2-), 96.96844 (H2PO4-), 147.04456 (C9H7O2-), 152.99547 (C3H6PO5-), 164.07146 (C9H10NO2-)	809.39862	120.08100 (C8H10N+), 292.11795 (C15H18NO5+), 310.12888 (C15H20NO6+), 328.26379 (C22H34NO+), 482.14206 (C18H29NPO12+)
	8.68	553.31519	78.95780 (PO3-), 209.02257 (C6H10PO6-)	555.32969	
GPE	8.71	684.33728	59.01253 (C2H3O2-), 71.01254 (C3H3O2-), 78.95777 (PO3-), 89.02324 (C3H5O3-), 96.96849 (H2PO4-), 101.02334 (C4H5O3-), 113.02348 (C5H5O3-), 119.03407 (C4H7O4-), 140.01114 (C2H7NPO4-), 152.99535 (C3H6PO5-), 171.00600 (C3H8PO6-), 196.03767 (C5H11NPO5-), 214.04849 (C5H13NPO6-), 333.05933 (C9H18PO11-), 376.10141 (C11H23NPO11-)		
	8.73	566.27405	78.95774 (PO3-), 140.01099 (C2H7NPO4-), 302.06439 (C8H17NPO9-)		
GPE	8.97	678.32660	59.01255 (C2H3O2-), 71.01257 (C3H3O2-), 78.95781 (PO3-), 89.02327 (C3H5O3-), 101.02337 (C4H5O3-), 113.02353 (C5H5O3-), 119.03414 (C4H7O4-), 140.01122 (C2H7NPO4-), 152.99541 (C3H6PO5-), 196.03793 (C5H11NPO5-), 214.048715041 (C11H23NPO11-)	680.34070	86.06062 (C4H8NO+), 346.27405 (C22H36NO2+)
GPE	9.01	684.41022	59.01252 (C2H3O2-), 71.01253 (C3H3O2-), 78.95779 (PO3-), 96.96846 (H2PO4-), 140.01132 (C2H7NPO4-), 152.99547 (C3H6PO5-), 171.00615 (C3H8PO6-), 214.04858 (C5H13NPO6-), 376.10132 (C11H23NPO11-), 652.30872 (C29H51NPO13-)	686.42472	
GPE	9.07	654.32684	59.01255 (C2H3O2-), 71.01257 (C3H3O2-), 78.95781 (PO3-), 89.02325 (C3H5O3-), 101.02335 (C4H5O3-), 113.02352 (C5H5O3-), 119.03412 (C4H7O4-), 140.01122 (C2H7NPO4-), 152.99545 (C3H6PO5-), 196.03806 (C5H11NPO5-), 214.04872 (C5H13NPO6-), 333.05911 (C9H18PO11-), 376.10132 (C11H23NPO11-)	656.34082	86.06062 (C4H8NO+), 322.27408 (C20H36NO2+)
GPE	9.08	682.39417	78.95781 (PO3-), 140.01123 (C2H7NPO4-), 152.99542 (C3H6PO5-), 171.00623 (C3H8PO6-), 214.04877 (C5H13NPO6-)	684.40867	
	9.24	726.25671			
GPE	9.36	478.25769	78.95780 (PO3-), 140.01129 (C2H7NPO4-), 152.99544 (C3H6PO5-), 171.00621 (C3H8PO6-), 214.04857 (C5H13NPO6-)	480.27219	
ascr	9.58	514.37555	73.02817 (C3H5O2-), 83.04894 (C5H7O-), 86.02350 (C3H4NO2-), 111.04424 (C6H7O2-), 297.28006 (C19H37O2-), 427.34241 (C25H47O5-)	516.39005, 538.37115	
	9.59	567.33087	78.95782 (PO3-), 96.96853 (H2PO4-)	569.34537	
ascr	9.86	576.41205	100.03931 (C4H6NO2-), 102.05501 (C4H8NO2-), 427.34274 (C25H47O5-), 512.39484 (C29H54NO6-)	532.42105	62.06082 (C2H8NO+), 366.33664 (C23H44NO2+), 384.34717 (C23H46NO3+), 402.35773 (C23H48NO4+)
EA	10.09	298.23895	57.03328 (C3H5O-), 86.02362 (C3H4NO2-), 211.20676 (C14H27O-)	300.25345	62.06085 (C2H8NO+), 86.06062 (C4H8NO+), 282.24265 (C17H32NO2+)
ascr	10.16	528.39063	57.03336 (C3H5O-), 59.01258 (C2H3O2-), 71.01260 (C3H3O2-), 73.02824 (C3H5O2-), 83.04904 (C5H7O-), 86.02357 (C3H4NO2-), 111.04421 (C6H7O2-), 311.29575 (C20H39O2-), 441.35840 (C26H49O5-), 482.31137 (C26H44NO7-)	530.40513	62.06082 (C2H8NO+), 86.06062 (C4H8NO+), 364.32083 (C23H43NO2+), 382.33154 (C23H44NO3), 400.34213 (-130, C23H46NO4+)
ascr	10.49	542.40674	73.02822 (C3H5O2-), 83.04907 (C5H7O-), 86.02354 (C3H4NO2-), 111.04407 (C6H7O2-), 325.31116 (C21H41O2-), 455.37375 (C27H51O5-)	544.42124	62.06082 (C2H8NO+), 86.06062 (C4H8NO+), 353.30499 (C22H41O3+), 378.33673 (C24H44NO2+), 396.34735 (C24H46NO3+), 414.35809 (C24H48NO4+)
EA	10.69	324.25464	57.03329 (C3H5O-), 86.02351 (C3H4NO2-), 237.22223 (C16H29O-)	326.26914	62.06082 (C2H8NO+), 86.06059 (C4H8NO+), 308.25830

					(C19H34NO2+)
	10.70	387.25034			
EA	10.88	358.26022		314.26922	62.06087 (C2H8NO+), 86.06064 (C4H8NO+), 296.25848 (C18H34NO2+)
ascr	11.04	556.42255	73.02824 (C3H5O2-), 83.04900 (C5H7O-), 86.02356 (C3H4NO2-), 111.04422 (C6H7O2-), 339.32706 (C22H43O2-), 469.39001 (C28H53O5-)	558.43705	
	11.31	724.44159	78.95779 (PO3-), 96.96851 (H2PO4-), 140.01117 (C2H7NPO4-), 152.99538 (C3H6PO5-), 171.00610 (C3H8PO6-), 214.04857 (C5H13NPO6-)	726.45581	100.07612 (C5H10NO+), 424.37854 (C26H50NO3+)
ascr	11.55	616.44391	73.02824 (C3H5O2-), 83.04900 (C5H7O-), 86.02357 (C3H4NO2-), 111.04422 (C6H7O2-), 353.34253 (C23H45O2-), 483.40524 (C29H55O5-)	572.45291	62.06082 (C2H8NO+), 100.07610 (C5H10NON), 406.36783 (C26H48NO2+), 424.37854 (C26H50NO3+), 442.38919 (C26H52NO4+)
ascr	11.74	719.45984	57.03336 (C3H5O-), 59.01258 (C2H3O2-), 71.01260 (C3H3O2-), 73.02824 (C3H5O2-), 83.04904 (C5H7O-), 86.02357 (C3H4NO2-), 111.04421 (C6H7O2-), 381.33804 (C24H45O3-), 511.40027 (C30H55O6-)	692.49542, 697.45056	85.02898 (C4H5O2+), 113.05997 (C6H9O2+), 127.03905 (C6H7O3+), 131.07034 (C6H11O3+), 145.04958 (C6H9O4+), 291.30438 (C21H39+), 319.33578 (C23H43+), 329.32019 (C24H41+), 347.33072 (C24H43O+), 365.34137 (C24H45O2+)
ascr	12.37	644.47552	71.01260 (C3H3O2-), 73.02824 (C3H5O2-), 83.04904 (C5H7O-), 86.02357 (C3H4NO2-), 111.04421 (C6H7O2-), 381.37323 (C25H49O2-), 511.43613 (C31H59O5-)	600.48452	62.06082 (C2H8NO+), 100.07616 (C5H10NO+), 434.39944 (C28H52NO2+), 452.41019 (C28H54NO3+), 470.42041 (C28H56NO4+)
ascr	12.57	747.49164	57.03336 (C3H5O-), 59.01258 (C2H3O2-), 71.01260 (C3H3O2-), 73.02824 (C3H5O2-), 83.04904 (C5H7O-), 86.02357 (C3H4NO2-), 111.04421 (C6H7O2-), 409.36755 (C26H49O3-), 539.43164 (C32H59O6-)	720.52637, 725.48145	

Table S8. Differential metabolites from *C. elegans* L1 medium, ES+ mode, that are decreased or absent in N2 medium compared to *daf-22*. Peaks that are also in growth medium table (ES+) are shown in bold red. Entries that have a corresponding peak in the ES- table are shaded grey.

class	*rt (min)*	*m/z (ES+)*	*MS/MS (ES+)*	*m/z (ES-)*
GPE	1.08	488.04901	see L1s, ES- table	
GPE	1.13	325.99576	see L1s, ES- table	
	1.16	363.95160		
	3.08	268.66348		534.30521
	3.52	339.10535	177.05209 (C8H10O3Na+)	
	3.99	573.27435		
	4.02	345.70026	120.08106 (C8H10N+)	
	4.41	298.20035	136.06168 (C5H5N5+), 253.16586 (C12H21N4O2+)	
	4.68	330.22775	85.02892 (C4H5O2+), 144.10184 (C7H14NO2+), 151.1176 (C10H15O+), 169.12222 (C10H17O2+), 253.14336 (C14H21O4+), 271.15396 (C14H23O5+)	
	4.72	344.20703	60.08154 (C3H10N+), 85.02892 (C4H5O2+), 137.09604 (C9H13O+), 144.10184 (C7H14NO2+), 165.09099 (C10H13O2+), 201.11194 (C10H17O4+), 267.122256 (C14H19O5+), 285.13297 (C14H21O6+)	
	4.75	418.77179	112.08730 (C5H10N3+), 130.04994 (C5H8NO3+), 147.07623 (C5H11N2O3+), 183.14906 (C10H19N2O+), 226.67082 (z=2), 253.16588 (C12H21N4O2+), 289.19397, 331.73895 (z=2), 367.24518	834.52246
	4.76	374.25394	135.11681 (C10H15+), 153.12740 (C10H17O+), 297.16895 (C16H25O5+)	
	4.81	388.23331	121.10131 (C9H13+), 131.08559 (C10H11+), 144.10196 (C7H14NO2+), 149.09607 (C10H13O+), 167.10670 (C10H15O2+), 191.10678 (C12H15O2+), 293.13879 (C16H21O5+)	
	4.82	441.79276		
	5.03	354.74237		
	5.10	771.38885	127.08683 (C6H11N2O+), 341.14551 (C14H21N4O6+)	769.37435
	5.15	415.23047		427.21091, 437.23984
	5.17	413.21500		425.19565, 435.22421
	5.22	354.22522		366.20572, 376.23465
	5.60	285.25372	84.08130 (C5H10N+), 114.09156 (C6H12NO+), 143.11787 (C7H15N2O+)	
EA	5.63	362.25375	62.06079 (C2H8NO+), 290.21140 (C18H28NO2+), 308.22195 (C18H30NO3+), 326.23248 (C18H32NO4+), 344.24329 (C18H32NO5+)	360.23925
	5.64	830.47778	167.08136 (C8H11N2O2+), 185.12860 (C9H17N2O2+), 186.12352 (C8H16N3O2+), 212.10272 (C9H14N3O3+), 242.14987 (C11H20N3O3+), 311.17142 (C14H23N4O4+), 476.24997 (C23H34N5O6+)	828.46328
	5.65	416.26434	60.08151 (C3H10N+), 85.02892 (C4H5O2+), 177.12743 (C12H17O+), 195.13831 (C12H19O2+)	
	5.67	389.25345		
	5.72	378.24869	see L1s, ES- table	
EA	5.81	346.25888	62.06081 (C2H8NO+), 292.22690 (C18H30NO2+), 310.23761 (C18H32NO3+), 328.24811 (C18H34NO4+)	380.22134, 390.25034
	5.84	**212.20097**	see growth medium, ES+ table	
	5.92	452.24112	see L1s, ES- table	
	5.97	**213.18491**		229.18088
	5.98	403.26901	205.19522 (C15H25+), 223.20561 (C15H27O+), 241.21617 (C15H29O2+)	
	6.05	376.26947	see L1s, ES- table	
	6.08	226.21664	84.08131 (C5H10N+)	
	6.12	**211.16937**		
	6.14	380.24088	69.03419 (C4H5O+), 87.04450 (C4H7O2+), 183.17429 (C12H23O+); do MS/MS on 358.25894	356.24493, 392.22183
EA	6.14	**340.24838**	62.06080 (C2H8NO+), 86.06053 (C4H8NO+), 237.18478 (C15H25O2+), 279.19528 (C17H27O3+), 322.23740 (C19H32NO3+)	
EA	6.16	362.29004	62.06081 (C2H8NO+), 308.25858 (C19H34NO2+), 326.26901 (C19H36NO3+), 344.27939 (C19H38NO4+)	396.25222
	6.21	412.20975	see L1s, ES- table	
	6.23	**356.24313**	see growth medium, ES+ table	354.22863, 390.20596
	6.49	417.28479	219.21074 (C16H27+), 237.22116 (C16H29O+), 255.23122 (C16H31O2+)	
EA	6.54	**376.30569**	62.06078 (C2H8NO+), 322.27393 (C20H36NO2+), 340.28488 (C20H38NO3+), 358.29626 (C20H40NO4+)	410.26852
	6.65	386.19925	see L1s, ES- table	

	6.68	314.23239	60.05184 (C3H10N+), 85.02892 (C4H5O2+), 144.10190 (C7H14NO2+), 153.12735 (C10H17O+), 171.13786 (C10H19O2+), 255.15886 (C14H23O4+)	
	6.73	452.30060	85.02895 (C4H5O2+), 273.18436 (C18H25O2+), 375.21649 (C22H31O5+), 393.22708 (C22H33O6+)	
	6.79	**225.18486**		
	6.84	**316.24826**	60.08155 (C3H10N+), 85.02895 (C4H5O2+), 257.17453 (C14H25O4+)	
	6.90	492.23935	94.03932 (C4H7ONa+, rad), 139.02379 (C4H6NO3Na+, rad), 152.03181 (C5H7NO3Na+, rad), 162.10141 (C9H15ONa+, rad), 175.10938 (C10H16ONa+), 201.00661 (C5H8NSO4Na+, rad), 246.15909 (C14H23O2Na+, rad), 315.22937 (C19H32O2Na+), 331.22385 (C19H32O3Na+), 363.19620 (C19H32NSO3Na+)	468.24344
	6.99	490.22336	104.10735 (C5H14NO+), 173.09363 (C10H14ONa+), 244.14357 (C14H21O2Na+, rad), 313.21317 (C19H30O2Na+), 318.24271 (C20H32NO2+), 329.20874 (C19H30O3Na+), 361.18066 (C19H30OS3Na+)	466.22726
	7.13	310.23770	56.05031 (C3H6N+), 82.06567 (C5H8N+), 238.21642 (C15H28NO+), 250.21645 (C16H28NO+), 280.22687 (C17H30NO2+), 292.22681 (C18H30NO2+)	
	7.30	442.14282		418.14627
	7.38	374.29007	60.08155 (C3H10N+), 85.02895 (C4H5O2+), 144.10207 (C7H14NO2+), 159.06509 (C7H11O4+), 297.20575 (C17H29O4+), 315.21606 (C17H31O5+)	
	7.44	381.18024		
	7.47	526.20038		502.20398
	7.47	291.19290		
	7.54	434.26682	60.08155 (C3H10N+), 85.02895 (C4H5O2+), 291.17218 (C15H28O3Cl+)	
	7.56	263.20047		
	7.60	347.21927		
	7.62	239.20047		
	7.63	410.29007		
	7.65	355.24802		353.23352
	7.72	594.29626	60.08156 (C3H10N+), 71.07362 (C4H9N+, rad), 86.09695 (C5H12N+), 104.10733 (C5H14NO+), 124.99993 (C2H6PO4+), 184.07332 (C5H15NPO4+)	
	7.75	253.21611		
	7.81	311.13843		
	8.08	325.15414		
	8.09	307.22687		
	8.34	322.21442	215.17961 (C16H23+), 233.19017 (C16H25O+), 269.16653 (C16H26OCl+), 287.17709 (C16H28O2Cl+)	
	8.37	336.25333	62.06080 (C2H8NO+), 142.08620 (C7H12NO2+), 229.19518 (C17H25+), 257.18985 (C18H25O+), 275.20068 (C18H27O2+), 318.24252 (C20H32NO2+)	
	8.39	351.14899		
	8.45	277.25278		
	8.48	644.34147	see L1s, ES- table	
	8.56	476.24466	139.02397 (C4H6NO3Na+, rad), 152.03172 (C5H7NO3Na+), 184.00375 (C5H7NSO3Na+), 201.00694 (C5H8NSO4Na+, rad), 297.21893 (C19H30ONa+), 299.23489 (C19H32ONa+), 304.26306 (C20H34NO+), 315.22910 (C19H32O2Na+), 347.20117 (C19H32SO2Na+)	452.24811
	8.61	516.30872	see L1s, ES- table	
	8.62	528.30847	60.08155 (C3H10N+), 86.09694 (C5H12N+), 104.10733 (C5H14NO+), 124.99994 (C2H6PO4+), 184.07327 (C5H15NPO4+)	526.29397
	8.62	492.30853	60.08155 (C3H10N+), 86.09694 (C5H12N+), 104.10733 (C5H14NO+), 124.99994 (C2H6PO4+), 184.07327 (C5H15NPO4+)	
	8.67	416.37360		
	8.92	325.23730	271.20544 (C19H27O+), 289.21613 (C19H29O2+), 307.22672 (C19H31O3+)	
	8.99	331.22424		
	9.09	542.32428	60.08155 (C3H10N+), 86.09694 (C5H12N+), 104.10733 (C5H14NO+), 124.99994 (C2H6PO4+), 184.07327 (C5H15NPO4+)	
	9.14	506.32422	60.08155 (C3H10N+), 86.09694 (C5H12N+), 104.10733 (C5H14NO+), 124.99994 (C2H6PO4+), 184.07327 (C5H15NPO4+)	
	9.15	787.42712	85.02894 (C4H5O2+), 134.03667 (C5H9NOCl+)	
	9.16	530.32452	60.08155 (C3H10N+), 86.09694 (C5H12N+), 104.10733 (C5H14NO+), 124.99994 (C2H6PO4+), 184.07327 (C5H15NPO4+)	
	9.27	512.39478	85.02897 (C4H5O2+), 144.10190 (C7H14NO2+), 305.28433 (C21H37O+), 369.30002 (C22H41O4+), 407.31534 (C25H43O4+), 435.30972 (C26H43O5+)	
	9.35	616.47864	60.08154 (C3H10N+), 85.02895 (C4H5O2+), 104.10737 (C5H14NO+), 113.06002 (C6H9O2+), 144.10196 (C7H14NO2+), 409.33038 (C25H45O4+), 486.41678 (C28H56NO5+)	
	9.41	481.34991		
	9.43	365.18530		
	9.43	633.42395	60.08154 (C3H10N+), 85.02893 (C4H5O2+), 134.03668 (C5H9NOCl+)	
	9.51	544.33984	60.08155 (C3H10N+), 86.09694 (C5H12N+), 104.10732 (C5H14NO+), 124.99992 (C2H6PO4+), 184.07329 (C5H15NPO4+)	
	9.54	498.41559	85.02897 (C4H5O2+), 144.10196 (C7H14NO2+), 319.30029 (C22H39O+), 421.33096	

			(C26H45O4+), 439.34210 (C26H47O5+)	
	9.55	514.41064	60.08154 (C3H10N+), 85.02893 (C4H5O2+), 144.10188 (C7H14NO2+), 307.29919 (C21H39O+), 335.29385 (C22H39O2+), 371.31561 (C22H43O4+), 437.32651 (C26H45O5+)	
	9.60	532.34027	60.08157 (C3H10N+), 86.09695 (C5H12N+), *104.10734 (C5H14NO+), 124.99996 (C2H6PO4+), 184.07332 (C5H15NPO4+), (* big in 2nd peak, which may be indicative of 1-acyl-lysoPC regioisomer, JACS, 1996, 118, 451; this elution order, sn-2 first, is consistent with literature, Lipids, 1985, 20, 922)	
	9.63	*526.41052 ?*		
	9.66	614.46283	60.08158 (C3H10N+), 104.10739 (C5H14NO+), 144.10191 (C7H14NO2+)	
	9.69	520.34003	60.08157 (C3H10N+), 86.09695 (C5H12N+), *104.10734 (C5H14NO+), 124.99996 (C2H6PO4+), 184.07332 (C5H15NPO4+), (* big in 2nd peak, which may be indicative of 1-acyl-lysoPC regioisomer, JACS, 1996, 118, 451; this elution order, sn-2 first, is consistent with literature, Lipids, 1985, 20, 922)	
	9.92	528.42584	60.08157 (C3H10N+), 85.02896 (C4H5O2+), 144.10199 (C7H14NO2+), 321.31601 (C22H41O+), 349.31030 (C23H41O2+), 385.33112 (C23H45O4+), 451.34134 (C27H47O5+)	
	9.93	495.36581		
	9.93	644.50989	60.08154 (C3H10N+), 85.02896 (C4H5O2+), 113.06007 (C6H9O2+), 144.10202 (C7H14NO2+), 437.36246 (C27H49O4+), 514.44727 (C30H60NO5+)	
	9.96	973.62537		971.61087
	9.96	508.34021	60.08157 (C3H10N+), 86.09695 (C5H12N+), *104.10734 (C5H14NO+), 124.99996 (C2H6PO4+), 184.07332 (C5H15NPO4+), (* big in 2nd peak, which may be indicative of 1-acyl-lysoPC regioisomer, JACS, 1996, 118, 451; this elution order, sn-2 first, is consistent with literature, Lipids, 1985, 20, 922)	
	9.97	570.47314	85.02893 (C4H5O2+)	
	10.06	540.42590	85.02893 (C4H5O2+)	
	10.16	546.35553	60.08157 (C3H10N+), 86.09695 (C5H12N+), *104.10734 (C5H14NO+), 124.99996 (C2H6PO4+), 184.07332 (C5H15NPO4+), (* big in 2nd peak, which may be indicative of 1-acyl-lysoPC regioisomer, JACS, 1996, 118, 451; this elution order, sn-2 first, is consistent with literature, Lipids, 1985, 20, 922)	
	10.16	656.50995	60.08160 (C3H10N+), 85.02898 (C4H5O2+), 113.06004 (C6H9O2+), 144.10196 (C7H14NO2+), 347.33063 (C24H43O+), 365.34119 (C24H45O2+), 449.36194 (C28H49O4+), 467.37344 (C28H51O5+), 526.44751 (C31H60NO5+)	
	10.18	702.55139	60.08155 (C3H10N+), 85.02898 (C4H5O2+), 113.06006 (C6H9O2+), 144.10207 (C7H14NO2+), 572.48853 (C33H66NO6+)	
	10.21	542.44220	60.08157 (C3H10N+), 85.02896 (C4H5O2+), 437.36276 (C27H49O4+)	
	10.29	526.44684	85.02897 (C4H5O2+)	
	10.29	658.52570	85.02896 (C4H5O2+), 113.05994 (C6H9O2+), 528.46271 (C31H62NO5+)	
	10.37	265.21613		
	10.41	554.44147	85.02898 (C4H5O2+)	
	10.62	556.45764	1st peak (10.6 min): 60.08154 (C3H10N+), 85.02895 (C4H5O2+); 2nd and 3rd peaks (12.3 and 12.6 min): 62.06079 (C2H8NO+), *319.33685 (C23H43+), 347.33087 (C24H43O+), *365.34143 (C24H45O2+), 408.38336 (C26H50NO2+), *409.36661 (C26H49O3+), 426.39410 (C26H52NO3+); (* only in 12.6 min peak)	
	10.66	672.54175	60.08157 (C3H10N+), 85.02895 (C4H5O2+), 113.05993 (C6H9O2+), 144.10181 (C7H14NO2+), 542.47760 (C32H64NO5+)	
	10.72	684.54169	85.02895 (C4H5O2+), 113.05996 (C6H9O2+), 375.36206 (C26H47O+), 477.39417 (C30H53O4+), 554.47809 (C33H64NO5+)	
	10.78	430.38940	62.06081 (C2H8NO+), 394.36786 (C25H48NO2+), 412.37866 (C25H50NO3+)	
	10.78	582.43451		
	10.84	686.55780	85.02895 (C4H5O2+), 113.06007 (C6H9O2+), 479.41135 (C30H55O4+), 556.49463 (C33H66NO5+)	
	10.93	554.47858	85.02898 (C4H5O2+), *477.39398 (C30H53O4+); (* only 1st peak)	
	11.06	552.46289	85.02895 (C4H5O2+)	
	11.16	496.24652		494.23202
	11.26	478.35092	see L1s, ES- table	
	11.35	596.45032		
	11.35	700.57288	60.08157 (C3H10N+), 85.02895 (C4H5O2+), 113.06003 (C6H9O2+), 144.10194 (C7H14NO2+), 570.50946 (C33H68NO6+)	
	11.41	596.39307	see L1s, ES- table	
	11.54	572.45306	62.06083 (C2H8NO+), 100.07604 (C5H10NO+), 406.36789 (C26H48NO2+), 424.37833 (C26H50NO3+), 442.38989 (C26H52NO4-)	606.41524
	11.74	492.36652		468.37036
	11.86	440.37399	1st peak: 62.06079 (C2H8NO+), 100.07607 (C5H10NO+), 305.28406 (C21H37O+), 323.29443 (C21H39O2+), 341.30490 (C21H41O3+), 353.34052 (C23H45O2+), 379.32086 (C24H43O3+), 422.36273 (C26H48NO3+); 2nd peak: 62.06079 (C2H8NO+), 112.07593 (C6H10NO+), 315.30515 (C23H39+), 333.31534 (C23H41O+), 361.30966 (C24H41O2+), 376.35749 (C25H46NO+), 379.32065 (C24H43O3+), 397.33087 (C24H45O4+), 404.35217 (C26H46NO2+), 422.36282 (C26H48NO3+)	438.35949

	11.94	610.46613		622.44656
	12.10	472.43677	62.06081 (C2H8NO+), 88.03981 (C3H6NO2+), 436.41513 (C28H54NO2+), 454.42581 (C28H56NO3+)	636.46218
	12.20	553.40826		529.41180
	12.23	490.33005	134.03671 (C5H9NOCl+), 357.29968 (C21H41O4+), 454.30786 (C26H45NO3Cl+), 472.31897 (C26H47NO4Cl+)	488.31583
	12.29	585.38977		
	12.30	410.36310	303.30453 (C22H39+), 321.31506 (C22H41O+), 392.35214 (C25H46NO2+)	
	12.31	426.39438	62.06079 (C2H8NO+), 291.30429 (C21H39+), 319.33661 (C23H43+), 329.32117 (C24H41+), 347.33054 (C24H43O+), 365.34131 (C24H45O2+), 408.38379 (C26H50NO2+), 409.36792 (C29H49O3+)	590.41982
	12.36	600.48389	see L1s, ES- table	
	12.38	628.39502		
	12.63	509.38187		
	12.71	567.42358	see L1s, ES- table	
EA	12.80	468.40546	62.06079 (C2H8NO+), 100.07603 (C5H10NO+), 333.31436 (C23H41O+), 351.32611 (C23H43O2+), 369.33624 (C23H45O3+), 381.37213 (C25H49O2+), 407.35168 (C26H47O3+), 450.39398 (C28H52NO3+)	502.36764
	12.80	476.35062	70.02942 (C3H4NO+), 88.03979 (C3H6NO2+), 134.03677 (C5H9NOCl+), 317.32022 (C23H41+), 335.33087 (C23H43O+), 404.35272 (C26H46NO2+), 422.36301 (C26H48NO3+), 440.32919 (C26H47NO2Cl+), 458.34283 (C26H49NO3Cl+)	
	13.05	581.43933		557.44293
	13.09	353.34134	317.32022 (C23H41+), 335.33044 (C23H43O+)	
	13.10	603.33820		
	13.13	638.49731		650.47768
	13.15	504.40286		
	13.17	527.34802		
	13.18	551.42889		
	13.25	493.38693		
	13.28	504.38174	70.02940 (C3H4NO+), 88.03978 (C3H6NO2+), 134.03679 (C5H9NOCl+), 345.35110 (C25H45+), 363.36221 (C25H47O+), 432.38382 (C28H50NO2+), 450.39468 (C28H52NO3+), 468.36044 (C28H51NO2Cl+), 486.37119 (C28H53NO3Cl+)	
	13.28	656.42676	see L1s, ES- table	
	13.34	650.49725		
	13.37	535.39728		
	13.39	584.48938	62.06081 (C2H8NO+), *357.35150 (C26H45+), *375.36185 (C26H47O+), 436.41486 (C28H54NO2+), 454.42551 (C28H56NO3+); (* only in 2nd peak)	618.45156, 628.48253
	13.57	524.34839		
	13.66	567.46021		579.44049
	13.69	595.45520		571.45880
	13.69	507.40268		
	13.76	474.39240		
	13.96	516.42682	83.4968 (C5H7O+), 95.04945 (C6H7O+), 113.05993 (C6H9O2+), 173.08064 (C8H13O4+), 309.31577 (C21H41O+)	
	14.05	620.48651		
	14.07	573.41089	443.34735 (C24H47N2O5+), 499.37436 (C27H51N2O6+)	
	14.16	521.41827		
	14.39	621.38745	455.34692 (C25H47N2O5+), 511.37341 (C28H51N2O6+)	
	14.46	563.42859		
	14.53	537.41296		
	14.59	587.42651	457.36313 (C25H49N2O5+), 513.38989 (C28H53N2O6+)	
	14.75	535.43359		
	14.91	583.41003		595.39031
	14.95	549.41284		
	15.34	601.44214	471.37805 (C26H51N2O5+), 527.40527 (C29H55N2O6+)	
	15.38	549.44940		
	15.81	565.44421		
	15.97	605.43939	see L1s, ES- table	
	16.10	563.46521		
	16.32	577.44434		
	16.47	615.43896	313.21350 (C19H30O2Na+), 325.21384 (C20H30O2Na+)	591.44256
	17.23	577.48041		
	17.34	591.43872	289.21381 (C17H30O2Na+), 325.21375 (C20H30O2Na+)	
	18.10	723.57501		735.55529
	18.18	591.49634		

Table S9. Differential metabolites from *C. elegans* growth medium, ES+ mode, that are decreased or absent in N2 medium compared to *daf-22*. Peaks that are also in L1 medium table (ES+) are shown in bold red. Entries that have a corresponding peak in the ES- table are shaded grey.

class	*rt (min)*	*m/z (ES+)*	*MS/MS (ES+)*	*m/z (ES-)*
	1.46	215.21187	70.06580 (C4H8N+), 84.08130 (C5H10N+), 86.09692 (C5H12N+), 98.09679 (C6H12N+), 103.12328 (C5H15N2+), 115.12318 (C6H15N2+), 198.18523 (C12H24NO+)	
	2.18	221.04144	193 00987 (C5H9N2S2O2+)	
	4.18	269.22241	100.07607 (C5H10NO+), 169.13344 (C9H17N2O+)	
	4.80	431.12869	99.05568 (C4H7N2O+), 142.08632 (C7H12NO2+), 144.08078 (C10H10N+), 171.09138 (C11H11N2+), 251.11852 (C16H15N2O+), 339.13470 (C19H19N2O4+), 343.11182 (C18H19N2SO3+), 389.11661 (C19H21N2SO5+)	
	4.87	320.27966	60.04518 (C2H6NO+), 266.24756 (C17H32NO+), 284.25821 (C17H34NO2+), 302.26874 (C17H36NO3+)	
	5.02	249.13449	105.03378 (C7H5O+), 137.04578 (C5H5N4O+)	
	5.67	**212.20111**	84.08130 (C5H10N+)	
EA	5.69	218.17520	62.06082 (C2H8NO+), 182.15390 (C11H20NO+), 183.13797 (C11H19O2+), 200.16452 (C11H22NO2+)	252.13738, 262.16626
	5.83	458.25159	86.06059 (C4H8N+), 98.06049 (C5H8NO+), 250.21637 (C16H28NO+), 268.22693 (C16H30NO2+), 286.23761 (C16H32NO3+)	456.23679
EA	5.92	360.27460	62.06084 (C2H8NO+), 306.24261 (C19H32NO2+), 324.25323 (C19H34NO3+), 342.26385 (C19H36NO4+)	394.23678, 404.26605
	5.94	**213.18507**		
	5.94	216.15970	see growth medium, ES- table	
	5.94	296.25851	first two peaks: 84.08133 (C5H10N+); third peak: 70.06580 (C4H8N+)	
	6.09	**211.16954**		
	6.11	**340.24866**	see L1, ES+ table	
EA	6.22	390.28503	62.06081 (C2H8NO+), 318.24298 (C20H32NO2+), 336.25311 (C20H34NO3+), 354.26340 (C20H36NO4+), 372.27420 (C20H38NO5+)	388.27053
	6.26	**356.24326**	60.08157 (C3H10N+), 85.02896 (C4H5O2+), 213.07552 (C10H13O5+), 297.16946 (C16H25O5+)	
EA	6.28	372.27454	see growth medium, ES- table	
EA	6.35	**376.30582**	see L1, ES+ table	410.26816, 420.29709
GPE	6.39	662.35211	86.06057 (C4H8NO+), 292.26315 (C19H34NO+), 310.27393 (C19H36NO2+), 328.28430 (C19H38NO3+)	660.33761
EA	6.40	388.26953	62.06081 (C2H8NO+), 86.06059 (C4H8NO+), 249.18483 (C16H25O2+), 291.19537 (C18H27O3+), 309.20581 (C18H29O4+), 334.23749 (C20H32NO3+), 352.24820 (C20H34NO4+), 370.25839 (C20H36NO5+)	386.25528
	6.42	435.21460	see growth medium, ES- table	
GPE	6.44	672.33612	see growth medium, ES- table	
GPE	6.50	660.33594	see growth medium, ES- table	
EA	6.54	300.25317	62.06081 (C2H8NO+), 282.24252 (C17H32NO2+)	
EA	6.54	374.28995	62.06081 (C2H8NO+), 86.06056 (C4H8NO+), 277.21600 (C18H29O2+), 295.22662 (C18H31O3+), 320.25821 (C20H34NO2+), 338.26865 (C20H36NO3+), 356.27927 (C20H38NO4+)	372.27545, 408.25259
EA	6.57	304.24826	see growth medium, ES- table	
	6.60	514.37439	84.08134 (C5H10N+), 352.32108 (C22H42NO2+), 384.34674 (C23H46NO3+)	
GPE	6.63	648.33557	see growth medium, ES- table	
	6.68	384.31094	first two peaks: 84.08134 (C5H10N+); third peak: 62.06083 (C2H8NO+), 86.06061 (C4H8NO+), 299.25803 (C18H35O3+), 323.25809 (C20H35O3+), 366.30029 (C22H40NO3+)	
	6.69	392.31598	84.08132 (C5H10N+)	
	6.70	310.27408	84.08134 (C5H10N+)	
	6.76	**225.18495**		
EA	6.78	**316.24820**	see growth medium, ES- table	314.23407
	6.83	321.20358	see growth medium, ES- table	
	6.85	394.27994	179.17934 (C13H23+), 197.18999 (C13H25O+)	
	6.86	492.31693	see growth medium, ES- table	
GPE	6.88	674.35205	see growth medium, ES- table	
EA	6.92	398.29037	see growth medium, ES- table	
	6.96	352.28479	84.08133 (C5H10N+)	
	7.00	330.26389	62.06081 (C2H8NO+), 86.06056 (C4H8NO+), 294.24258 (C18H32NO2+), 312.25308 (C18H34NO3+)	8.1 min peak has HCl (364.22607)

				and FA (374.25500) adducts in ES-
	7.03	638.37524	see growth medium, ES- table	
	7.07	318.26389	see comments	
	7.08	324.28989	first two peaks have only 84.08130 (C5H10N+), third peak has only 70.06583 (C4H8N+)	
	7.13	396.27466	see growth medium, ES- table	
	7.18	336.28970	84.08128 (C5H10N+)	
	7.20	550.35095	70.06580 (C4H8N+), 84.08132 (C5H10N+), 340.32089 (C21H42NO2+)	
	7.21	389.20892	see growth medium, ES- table	
	7.24	385.25861		419.22079, 429.24957
	7.25	610.38037		
GPE	7.32	756.44116	see growth medium, ES- table	
	7.37	325.23749		359.19967, 369.22858
	7.39	640.39105	85.02896 (C4H5O2+), 127.03909 (C6H7O3+), 145.04955 (C6H9O4+), 245.22630 (C18H29+), 263.23669 (C18H31O+), 281.24734 (C18H33O2+), 325.11313 (C12H21O10+), 389.26929 (C24H37O4+), 407.27963 (C24H39O5+)	621.35006
	7.41	493.27768	see growth medium, ES- table	
	7.44	548.28595	see growth medium, ES- table	
	7.45	239.20071		
	7.47	274.27393	7.55 min: 70.06580 (C4H8N+), 88.07617 (C4H10NO+), 102.09171 (C5H12NO+), 106.08656 (C4H12NO2+); 8.15 min: 60.04519 (C2H6NO+), 226.25287 (C15H32N+), 238.25284 (C16H32N+), 256.26331 (C16H34NO+)	
	7.54	263.20059		
	7.58	564.36646	*70.06580 (C4H8N+), 84.08133 (C5H10N+), 354.33646 (C22H44NO2+); (* only in 2nd peak)	
	7.61	356.27948	7.6 min: 62.06080 (C2H8NO+), 320.25815 (C20H34NO2+), 338.26871 (C20H36NO3+); 7.9 min: 60.08157 (C3H10N+), 85.02895 (C4H5O2+), 144.10190 (C7H14NO2+), 157.04950 (C7H9O4+), 297.20569 (C17H29O4+); 8.4, 9.7 min - see growth medium, ES- table	354.26508 (8.4 and 9.7 min peaks)
GPE	7.63	676.36749	see growth medium, ES- table	
GPE	7.68	694.32031	see growth medium, ES- table	
	7.72	271.22681	171.13783 (C10H19O2+), 235.20549 (C16H27O+), 253.21591 (C16H29O2+)	
EA	7.74	340.24826	62.06082 (C2H8NO+), 237.18471 (C15H25O2+), 261.18457 (C17H25O2+), 279.19531 (C17H27O3+), 322.23746 (C19H32NO3+)	374.21063
	7.77	446.31137		
EA	7.78	332.27942	62.06082 (C2H8NO+), 149.05975 (C9H9O2+), 296.25830 (C18H34NO2+), 314.26886 (C18H36NO3+)	366.24173, 376.27060
	7.78	711.38306	70.06581 (C4H8N+), 86.06056 (C4H8NO+), 112.03960 (C5H6NO2+), 308.25818 (C19H34NO2+)	709.36856
	7.81	805.37469	see growth medium, ES- table	
	7.88	671.35181	see growth medium, ES- table	
	7.94	616.30975	see growth medium, ES- table	
	7.95	790.36395	98.06042 (C5H8NO+), 100.07605 (C5H10NO+), 126.05504 (C6H8NO2+), 137.04576 (C5H5N4O+), 320.25818 (C20H34NO2+), 456.29672 (C25H38N5O3+), 610.29980 (C28H45N5PO8+), 628.31067 (C28H47N5PO9+)	788.34945
	8.03	382.29504	see growth medium, ES- table	
	8.07	725.39880	84.08131 (C5H10N+), 86.06054 (C4H8NO+), 308.25815 (C19H34NO2+), 480.27219 (C22H43NPO8+)	723.38430
	8.12	287.25809	233.22635 (C17H29+), 251.23686 (C17H31O+), 269.24741 (C17H33O2+)	
	8.17	380.27948	62.06082 (C2H8NO+), 283.20547 (C20H27O+), 301.21603 (C20H29O2+), 326.24811 (C22H32NO+), 344.25812 (C22H34NO2+), 362.26947 (C22H36NO3+)	378.26498, 414.24222
	8.22	448.32715		
EA	8.24	328.24817	62.06081 (C2H8NO+), 207.17445 (C14H23O+), 225.18495 (C14H25O2), 243.19543 (C14H27O3+), 249.18501 (C16H25O2+), 267.19543 (C16H27O3+), 310.23758 (C18H32NO3+)	326.23367, 362.21100
	8.26	644.34088	see growth medium, ES- table	
	8.27	682.28717		
	8.27	688.30420		
	8.29	656.34082	see growth medium, ES- table	
	8.32	654.32550	see growth medium, ES- table	
	8.32	285.24231	231.21075 (C17H27+), 249.22121 (C17H29O+), 267.23169 (C17H31O2+)	
	8.39	308.25827	86.06059 (C4H8NO+)	
	8.39	642.32513	see growth medium, ES- table	
	8.57	300.25327	8.6 min: 187.13293 (C10H19O3+), 223.20592 (C15H27O+), 229.29560 (C17H25+), 247.20572 (C17H27O+), 265.21622 (C17H29O2+); 10.1 min: see growth medium, ES- table	
	8.59	409.34219	84.08136 (C5H10N+), 326.26907 (C19H36NO3+)	

	8.62	630.32532	86.06063 (C4H8NO+), 296.25845 (C18H34O2N+)	628.31082
	8.64	809.39862	see growth medium, ES- table	
	8.68	785.39844	120.08100 (C8H10N+), 166.08617 (C9H12NO2+), 292.11777 (C15H18NO5+), 304.26337 (C20H34NO+), 310.12827 (C15H20NO6+), 482.14243 (C18H29NPO12+)	783.38394
	8.68	606.41333	1st peak: 84.08137 (C5H10N+), 396.38370 (C25H50NO2+); 2nd and 3rd peaks additionally have 70.06584 (C4H8N+)	
	8.82	281.24744	199.16922 (C12H23O2+), 245.22639 (C18H29+), 263.23706 (C18H31O+)	
	8.90	309.24228	255.21057 (C19H27+), 273.22134 (C19H29O+), 291.23181 (C19H31O2+)	
	8.92	680.34070	see growth medium, ES- table	
	9.06	482.28787	86.06061 (C4H8NO+), 98.06048 (C5H8NO+), 292.26331 (C19H34NO+), 310.27390 (C19H36NO2+)	
	9.16	389.26617	371.25580 (C22H36O3Na+)	
	9.17	620.42926	1st peak: 84.08136 (C5H10N+), 410.39923 (C26H52NO2+) in MS/MS; 2nd peak additionally has 70.06589 (C4H8N+)	
	9.27	526.44696	1st peak: 84.08138 (C5H10N+), 396.38397 (C25H50NO2+); 2nd peak additionally has 70.06586 (C4H8N+), 200.12827 (C10H18NO3+)	
ascr	9.31	518.40570	62.06084 (C2H8NO+), 352.32092 (C22H42NO2+), 370.33163 (C22H44NO3+), 388.34225 (C22H46NO4+)	552.36788
	9.32	460.36319	277.25278 (C19H33O+), 295.26318 (C19H35O2+), 313.27374 (C19H37O3+)	
EA	9.35	360.31064	62.06087 (C2H8NO+), 306.27951 (C20H36NO+), 324.29004 (C20H38NO2+), 342.30054 (C20H40NO3+)	394.27282, 404.30197
ascr	9.45	540.46173	9.05 min: 56.05032 (C3H6N+), 84.08134 (C5H10N+), 214.14383 (C11H20NO3+), 410.39905 (C26H52NO2+); 9.30 min: 70.06588 (C4H8N+), 126.09155 (C7H12NO+), 200.12823 (C10H18NO3+), 410.39905 (C26H52NO2+)	
	9.51	584.28577	124.03950 (C6H6NO2+), 215.17972 (C16H23+), 268.08145 (C12H14NO6+)	618.24795, 628.27679
	9.54	227.20056		
	9.56	307.22684	271.20648 (C19H27O+), 289.21625 (C19H29O2+)	
ascr	9.62	516.38965	62.06082 (C2H8NO+), 86.06058 (C4H8NO+), *325.27368 (C20H37O3+), 350.30515 (C22H40NO2+), 368.31589 (C22H42NO3+), 386.32648 (C22H44NO4+)	514.37515, 550.35229, 560.38098
ascr	9.89	532.42084	see growth medium, ES- table	
ascr	10.16	530.40533	see growth medium, ES- table	
ascr	10.20	488.39459	305.28369 (C21H37O+), 323.29449 (C21H39O2+), 341.30518 (C21H41O3+)	
	10.44	568.41901		580.39929
ascr	10.49	544.42126	see growth medium, ES- table	
EA	10.53	398.32681	62.06086 (C2H8NO+), 86.06065 (C4H8NO+), 277.25314 (C19H33O+), 295.26285 (C19H35O2+), 313.27380 (C19H37O3+), 337.27383 (C21H37O3+), 380.31607 (C23H42NO3+)	396.31231, 432.28900
EA	10.69	326.26892	see growth medium, ES- table	
	10.70	337.30994	241.21593 (C15H29O2+), 255.23206 (C16H31O2+)	
ascr	10.71	502.41043	319.29962 (C22H39O+), 337.31009 (C22H41O2+), 355.32086 (C22H43O3+)	
	10.78	726.45581	see growth medium, ES- table	
ascr	10.79	560.45282	62.06082 (C2H8NO+), 376.35785 (C25H46NO+), 394.36826 (C25H48NO2+), 412.37866 (C25H50NO3+), 430.38922 (C25H52NO4+)	594.41500
	10.83	440.37372	11.9 min: 62.06082 (C2H8NO+), 325.27362 (C20H37O3+), 341.30457 (C21H41O3+), 379.32086 (C24H43O3+), 422.36288 (C26H48NO3+); 12.2 min: 62.06082 (C2H8NO+), 325.27362 (C20H37O3+), 355.32077 (C22H43O3+), 379.32089 (C24H43O3+), 422.36288 (C26H48NO3+)	474.33590
	10.85	271.26315	235.24219 (C17H31+), 253.25266 (C17H33O+)	
	10.86	314.26892	see growth medium, ES- table	
	10.87	356.31577		
	10.97	364.28455		362.27005, 398.24695
	10.98	321.16650	57.07075 (C4H9+), 72.04508 (C3H6NO+), 100.07610 (C5H10NO+), 156.13837 (C9H18NO+)	
	11.05	410.36295	see comments	
	11.05	428.37366	see comments	
ascr	11.05	558.43689	62.06082 (C2H8NO+), 86.06058 (C4H8NO+), 392.35233 (C25H46NO2+), 410.36292 (C25H48NO3+), 428.37360 (C25H50NO4+)	556.42239, 592.39948, 602.42841
EA	11.07	412.34229	62.06082 (C2H8NO+), 86.06058 (C4H8NO+), 291.26816 (C20H35O+), 309.27890 (C20H37O2+), 327.28937 (C20H39O3+), 351.28943 (C22H39O3), 394.33188 (C24H44NO3+)	410.32779, 446.30466
EA	11.08	386.36292	62.06084 (C2H8NO+), 368.35291 (C23H46NO2+)	
	11.18	837.56104	84.08137 (C5H10N+), 124.99995 (C2H6PO4+), 184.07330 (C5H15NPO4+), 448.41574 (C29H54NO2+), 452.40942 (C28H54NO3+), 466.42560 (C29H56NO3+)	
	11.19	355.32080	241.21635 (C15H29O2+), 255.23204 (16H31O2+), 319.29941 (C22H39O+), 337.31000 (C22H41O2+)	
	11.21	267.26816		
EA	11.26	456.36841	62.06082 (C2H8NO+), 100.07612 (C5H10NO+), 282.27914 (C18H36NO+), 420.34659	454.35391

			(C26H46NON+), 438.35788 (C26H48NO4+)	
	11.29	454.35321		452.33871
ascr	11.30	574.46887	62.06082 (C2H8NO+), 390.37314 (C26H48NO+), 408.38394 (C26H50NO2+), 426.39426 (C26H52NO3+), 444.40503 (C26H54NO4+)	608.43105, 618.45966
	11.30	297.27896		
	11.31	516.42615		
	11.33	572.45239	see growth medium, ES- table	
EA	11.36	426.35803	all peaks have 62.06082 (C2H8NO+); additionally, 11.3 min peak has: 100.07618 (C5H10NO+), 291.26831 (C20H35O+), 309.27893 (C20H37O2+), 327.28998 (C20H39O3+), 365.30518 (C23H41O3+), 408.34741 (C25H46NO3+); 11.55 and 11.65 min peaks have: 305.28387 (C21H37O+), 323.29449 (C21H39O2+), 341.30521 (C21H41O3+), 365.30518 (C23H41O3+), 408.34741 (C25H46NO3+)	460.32021
	11.43	432.36838	249.25772 (C18H33+), 267.26819 (C18H35O+); 2nd peak additionally has 285.27869 (C18H37O2+)	
	11.45	528.42603	10.2 min: 85.02900 (C4H5O2+); 11.5 min: 325.27411 (C20H37O3+), 380.35272 (C24H46NO2+), 398.36301 (C24H48NO3+);	
	11.75	383.35223	see comments	
ascr	11.75	692.49512	see growth medium, ES- table	
	11.76	446.38440	263.27316 (C19H35+), 281.28372 (C19H37O+); 2nd peak additionally has 299.29459 (C19H39O2+)	
	11.78	384.34738	10.8 min: 62.06086 (C2H8NO+), 366.33691 (C23H44NO2+)	
	11.85	354.30032	see comments	
ascr	11.95	588.48413	62.06083 (C2H8NO+), 422.39948 (C27H52NO2+), 440.41019 (C27H54NO3+), 458.42047 (C27H56NO4+)	622.44631
	12.01	529.44714	345.35187 (C25H45+), 363.36212 (C25H47O+)	
	12.07	342.30042	62.06085 (C2H8NO+), 86.06064 (C4H8NO+), 324.28979 (C20H38NO2+)	
ascr	12.14	586.46857	62.06085 (C2H8NO+), 86.06064 (C4H8NO+), 420.38361 (C27H50NO2+), 438.39429 (C27H52NO3+)	584.45407, 620.43073
	12.18	544.45776	361.34659 (C25H45O+), 379.35718 (C25H47O2+)	
	12.29	460.40005	277.28925 (C20H37+), 295.29974 (C20H39O+); 2nd peak additionally has 313.31030 (C20H41O2+)	
ascr	12.36	600.48395	see growth medium, ES- table	
	12.40	694.51050	85.02903 (C4H5O2+), 95.04966 (C6H7O+), 97.02892 (C5H5O2+), 113.06007 (C6H9O2+), 127.03916 (C6H7O3+), 131.07059 (C6H11O3+), 145.04971 (C6H9O4+), 349.34668 (C24H45O+), 367.35727 (C24H47O2+)	675.47000
ascr	12.56	556.45764	347.33090 (C24H43O+), 408.38376 (C26H50NO2+), 426.39459 (C26H52NO3+)	590.41982
	12.57	393.37265	319.33627 (C23H43+), 347.36789 (C25H47+), 357.35144 (C26H45+), 375.36246 (C26H47O+)	
EA	12.62	454.38950	62.06085 (C2H8NO+), 282.27823 (C18H36NO+), 313.27383 (C19H37O3+), 369.33578 (C23H45O3+), 393.33575 (C25H45O3+), 436.37976 (C27H50NO3+)	488.35168
	12.79	474.41592	291.30457 (C21H39+), 309.31509 (C21H41O+); 2nd peak additionally has 327.32602 (C21H43O2+)	491.35210
	12.80	468.40509	62.06083 (C2H8NO+), 100.07610 (C5H10NO+), 212.23735 (C14H30N+), 407.35123 (C26H47O3+), 450.39441 (C28H52NO3+)	502.36727
	13.13	638.49823		
ascr	13.17	614.50000	62.06083 (C2H8NO+), 448.41498 (C29H54NO2+), 466.42572 (C29H56NO3+)	648.46218
	13.25	488.43124	305.32031 (C22H41+), 323.33087 (C22H43O+); 2nd (small) peak additionally has 341.34128 (C22H45O2+)	505.36742
	13.35	604.47888	319.33673 (C23H43+), 343.33636 (C25H43+), 361.34680 (C25H45O+), 379.35757 (C25H47O2+), 439.37784 (C27H51O4+)	
	13.37	513.41565	291.30432 (C21H39+), 319.33646 (C23H43+), 329.32016 (C24H41+), 347.33087 (C24H43O+), 365.34152 (C24H45O2+)	511.40115
ascr	13.41	584.48883	375.36240 (C26H47O-), 436.41498 (C28H54NO2+), 454.42575 (C28H56NO3+)	618.45101
	13.48	367.35699	331.33612 (C23H43+), 349.34692 (C24H45O+)	
	13.71	502.44693	319.33594 (C23H43+), 337.34634 (C23H45O+); 2nd (smaller) peak additionally has 355.35687 (C23H47O2+)	
	13.80	451.37576		
ascr	14.08	573.40991	443.34793 (C24H47N2O5+), 499.37332 (C27H51N2O6+)	
	14.18	516.46240	333.35147 (C24H45+), 351.36206 (C24H47O+)	533.39858
	14.41	411.38327	319.33615 (C23H43+), 347.36719 (C25H47+), 357.35162 (C26H45+), 375.36224 (C26H47O+)	
	14.74	530.47839	347.36725 (C25H47+), 365.37784 (C25H49O+)	547.41457

Table S10. Differential metabolites from *P. pcificus* J2 medium, ES- mode, that are decreased or absent in RS2770 *Ppa-daf-22* medium compared to RS2333. Peaks that are also differential in growth medium are shown in red. **Peaks that are also in growth medium table (ES-) are shown in bold red.** Entries that have a corresponding peak in the ES+ table are shaded grey.

class	*rt (min)*	*m/z (ES-)*	*MS/MS (ES-)*	*m/z (ES+)*	*MS/MS (ES+)*
S	1.88	**211.02846**	85.06466 (C5H9O-), 96.95895 (HSO4-), 113.05977 (C6H9O2-), 131.07054 (C6H11O3-)		
ascr	3.25	455.17737	59.01254 (C2H3O2-), 71.01258 (C3H3O2-), 73.02823 (C3H5O2-), 85.02842 (C4H5O2-), 89.02329 (C3H5O3-), 95.01269 (C5H3O2-), 99.04408 (C5H7O2-), 101.02346 (C4H5O3-), 111.04436 (C6H7O2-), 113.02366 (C5H5O3-), 119.03429 (C4H7O4-), 123.04444 (C7H7O2-), 147.06580 (C6H11O4-), 161.04538 (C6H9O5-), 247.11864 (C11H19O6-), 271.11862 (C13H19O6-)	433.16763	141.05225 (C5H10O3Na+), 153.05228 (C6H10O3Na+), 271.11508 (C11H20O6Na+)
S	3.37	225.04401	96.95898 (HSO4-), 99.08042 (C6H11O-), 145.08650 (C7H13O3-)		
S	3.39	304.08612	63.96114 (SO2-), 74.00572 (C2H4NS-), 84.04427 (C4H6NO-), 113.04217 (C6H9S-), 116.01666 (C4H6NSO-), 128.03465 (C5H6NO3-), 175.04324 (C7H11SO3-), 178.01779 (C5H8NSO4-)	306.10083	84.04501 (C4H6NO+), 85.06543 (C5H9O+), 88.03989 (C3H6NO2+), 99.02674 (C5H7S+), 112.03970 (C5H6NO2+), 113.04222 (C6H9S+), 130.05005 (C5H8NO3+), 159.04761 (C7H11SO2+), 264.09000 (C10H18NSO5+)
S	3.44	211.06465	79.95608 (SO3-), 96.95898 (HSO4-)		
ascr	3.59	469.19308	73.02822 (C3H5O2-), 113.05982 (C6H9O2-), 261.13406 (C12H21O6-)	442.22808, 447.18399	
S	3.61	401.11264	96.95898 (HSO4-), 159.10222 (C7H15O3-), 239.05933 (C8H15SO6-)		
ascr	3.80	567.19379	73.02823 (C3H5O2-), 85.02831 (C4H5O2-), 113.02360 (C5H5O3-), 115.00289 (C4H3O4-), 157.01384 (C6H5O6-), 175.02470 (C6H7O6-), 247.11874 (C11H19O6-), 405.14008 (C17H25O11-)	586.23486	95.01321 (C5H3O2+), 101.06010 (C5H9O2+), 113.02367 (C5H5O3+), 129.01836 (C5H5O4+), 141.01825 (C6H5O4), 159.02867 (C6H7O5+), 177.03935 (C6H9O6+), 259.08121 (C11H15O7+), 277.09183 (C11H17O8+)
ascr	4.03	483.20877	73.02829 (C3H5O2-), 127.07575 (C7H11O2-), 275.14987 (C13H23O6-)	456.24377, 461.19968	
	4.04	**305.16074**			
S	4.06	239.05952	96.95902 (HSO4-), 113.09630 (C7H13O-), 159.10231 (C8H15O3-)		
S	4.17	225.08032	79.95609 (SO3-), 96.95900 (HSO4-)		
ascr	4.88	971.35278	73.02822 (C3H5O2-), 89.02324 (C3H5O3-), 98.02367 (C4H4NO2-), 108.04457 (C6H6NO-), 134.02419 (C7H4NO2-), 152.03485 (C7H6NO3-), 194.04584 (C9H8NO4-), 309.12521 (C18H17N2O3-), 335.10327 (C19H15N2O4-), 583.22888 (C30H35N2O10-), 763.29364 (C36H47N2O16-)	927.36133	91.05466 (C7H7+), *103.05466 (C8H7+), *120.08099 (C8H10N+), 136.03931 (C7H6NO2+), *146.06007 (C9H8NO+), *156.08089 (C11H10N+), *174.09137 (C11H12NO+), *184.07573 (C12H10NO+), 190.04980 (C10H8NO3+), *202.08630 (C12H12NO2+), 218.04488 (C11H8NO4+), *220.09691 (C12H14NO3+), 236.05511 (C11H10NO5+), 320.14908 (C17H22NO5+), 355.12823 (C19H19N2O5+), 398.10840 (C17H20NO10+), 517.18182 (C25H29N2O10+); (* pasc fragments)
	5.00	716.22363	78.95781 (PO3-), 96.96853 (H2PO4-), 202.08760 (C12H12NO2-), 581.19043 (C26H34N2PO11-)	718.23773	105.07030 (C8H9+), 136.03941 (C7H6NO2+), 204.10208 (C12H14NO2+), 222.11256 (C12H16NO3+), 244.06053 (C13H10NO4+), 262.07135 (C13H12NO5+), 264.12283 (C14H18NO4+), 330.13318 (C18H20NO5+), 483.17391 (C25H27N2O8+)
ascr	5.15	560.19080	78.95779 (PO3-), 96.96849 (H2PO4-), 131.07065 (C6H11O3-), 209.02202 (C6H10PO6-), 341.10123 (C12H22PO9-), 460.17368 (C20H31NPO9-)	562.20532	101.02374 (C4H5O3+), 103.05464 (C8H7+), 120.08102 (C8H10N+), 146.06009 (C9H8NO+), 156.08087 (C11H10N+), 157.06494 (C11H9O+), 174.09135 (C11H12NO+), 184.07565 (C12H10NO+), 202.08633 (C12H12NO2+), 220.09686 (C12H14NO3+), 238.10753 (C12H16NO4+); all these fragments are present in pasc#9 and pasc#12

ascr	5.15	**674.26752**	59.01256 (C2H3O2-), 71.01263 (C3H3O2-), 73.02829 (C3H5O2-), 85.02847 (C4H5O2-), 89.02338 (C3H5O3-), 98.02378 (C4H4NO2-), 101.02347 (C4H5O3-), 113.02364 (C5H5O3-), 119.03419 (C4H7O4-), 143.03445 (C6H7O4-), 161.04530 (C6H9O5-), 179.05602 (C6H11O6-), 218.08229 (C12H12NO3-), 247.11867 (C11H19O6-), 448.19705 (C23H30NO8-), 466.20795 (C23H32NO9-)	647.30286	all fragments present in 562.20532 at 5.15 min plus 364.13898 (C18H20NO7+), 382.14948 (C18H24NO8+), 482.20206 (C23H32NO10+)
S	5.24	**267.09100**	96.95888 (HSO4-), 141.12782 (C9H17O-), 187.13380 (C10H19O3-)		
	5.24	292.11942	72.00786 (C2H2NO2-), 83.04914 (C5H7O-), 91.05427 (C7H7-), 100.07585 (C5H10NO-), 118.06535 (C8H8N-), 147.04471 (C9H7O2-), 164.07141 (C9H10NO2-), 230.11893 (C14H16NO2-), 248.12886 (C14H18NO3-), 274.10852 (C15H16NO4-)		
	5.27	**471.18762**	163.03978 (C9H7O3-), 165.01894 (C8H5O4-), 165.05537 (C9H9O3-), 166.02679 (C8H6O4-, rad), 167.03470 (C8H7O4-), 179.03488 (C9H7O4-), 180.04269 (C9H8O4-, rad), 181.05057 (C9H9O4-), 182.05832 (C9H10O4-, rad), 218.09476 (C13H14O3-, rad), 233.11826 (C14H17O3-), 234.08966 (C13H14O4-, rad), 235.09749 (C13H15O4-), 249.11313 (C14H17O4-), 250.12096 (C14H18O4-, rad), 264.13669 (C15H20O4-, rad), 265.14444 (C15H21O4-), 309.13449 (C16H21O6-), *427.19702 (C21H31O9-), 471.18695 (C22H31O11-); (* only in 1st peak)	490.22897	151.07538 (C9H11O2+), 153.05464 (C8H9O3+), 154.06242 (C8H10O3+, rad), 169.08591 (C9H13O3+), 182.05739 (C9H10O4+, rad), 185.08089 (C9H13O4+), 197.08086 (C10H13O4+, major), 293.13815 (C16H21O5+)
S	5.35	253.11151	79.95612 (SO3-), 96.95901 (HSO4-)		
ascr	5.38	688.28271	59.01256 (C2H3O2-), 71.01258 (C3H3O2-), 73.02824 (C3H5O2-), 85.02837 (C4H5O2-), 89.02328 (C3H5O3-), 98.02372 (C4H4NO2-), 101.02341 (C4H5O3-), 113.02357 (C5H5O3-), 119.03416 (C4H7O4-), 143.03459 (C6H7O4-), 161.04526 (C6H9O5-), 179.05591 (C6H11O6-), 218.08235 (C12H12NO3-), 261.13385 (C12H21O6-), 462.21432 (C24H32NO8-), 480.22482 (C24H34NO9-)	661.31818	same fragments as 647.30286 at 5.15 min plus 364.13910 (C18H22NO7+), 382.14957 (C18H24NO8+)
	5.40	**215.12897**	85.06469 (C5H9O-), 99.04407 (C5H7O2-), 115.07558 (C6H11O2-), 153.12808 (C10H17O-), 169.12312 (C10H17O2-), 197.11823 (C11H17O3-)		
ascr	5.41	763.29425	73.02823 (C3H5O2-), 98.02361 (C4H4NO2-), 108.04444 (C6H6NO-), 134.02399 (C7H4NO2-), 144.04491 (C9H6NO-), 152.03484 (C7H6NO3-), 188.03514 (C10H6NO3-), 189.06683 (C10H9N2O2-), 199.05116 (C11H7N2O2-), 201.06683 (C11H9N2O2-), 203.08258 (C11H11N2O2-), 215.04610 (C11H7N2O3-), 216.03011 (C11H6NO4-), 229.06178 (C12H9N2O3-), 291.11392 (C18H15N2O2-), 309.12399 (C18H17N2O3-), 317.09332 (C19H13N2O3-), 335.10379 (C19H15N2O4-, major), 353.11441 (C19H17N2O5-), 583.22955 (C30H35N2O10-), 601.24017 (C30H37N2O11-)	765.30865	pasc fragments (see 927.36133 at 4.88 min), 91.05470 (C7H7+), 190.04985 (C10H8NO3+), 218.04486 (C11H8NO4+), 236.05525 (C11H10NO5+), 320.14920 (C17H22NO5+), 355.12872 (C19H19N2O5+), 373.13925 (C19H21N2O6+), 473.19183 (C24H29N2O8+), 517.18237 (C25H29N2O10+)
ascr	5.49	528.16376	78.95781 (PO3-), 96.96856 (H2PO4-)		
	5.53	273.17105	2nd peak: 59.01262 (C2H3O2-), 115.03915 (C5H7O3-), 139.11220 (C9H15O-); 3rd peak: 59.01262 (C2H3O2-), 97.06483 (C6H9O-), 111.08069 (C7H11O-), 113.05997 (C6H9O2-), 115.03934 (C5H7O3-), 127.07571 (C7H11O2-), 129.09140 (C7H13O2-)		
ascr	5.71	542.18005	78.95781 (PO3-), 96.96856 (H2PO4-), 209.02205 (C6H10PO6-), 323.08972 (C12H20PO8-)	544.19452	pasc fragments (see 927.36133 at 4.88 min), 211.03664 (C6H12PO6+)
S	5.73	281.10651	96.95601 (HSO4-), 155.14384 (C10H19O-), 201.14964 (C11H21O3-)		
ascr	5.75	793.30481	73.02821 (C3H5O2-), 89.02323 (C3H5O3-), 92.04944 (C6H6N-), 136.03975 (C7H6NO2-), 173.07202 (C10H9N2O-), 179.05621 (C6H11O6-), 185.07213 (C11H9N2O-), 187.08789	749.31293	pasc fragments (see 927.36133 at 4.88 min), 91.05473 (C7H7+), 320.14941 (C17H22NO5+), 339.13391 (C19H19N2O4+), 357.14490

			(C11H11N2O-), 199.05144 (C11H7N2O2-), 247.11839 (C11H19O6-), 275.11951 (C18H15N2O-), 293.13028 (C18H17N2O2-), 319.10901 (C19H15N2O3-),337.11917 (C19H17N2O4-), 567.23480 (C30H35N2O9-), 585.24561 (C30H37N2O10-)		(C19H21N2O5+), 483.17523 (C25H27N2O8+), 501.18668 (C26H29N2O9+)
ascr	5.93	927.31812	73.02818 (C3H5O2-), 78.95779 (PO3-), 96.96849 (H2PO4-), 108.04451 (C6H6NO-), 148.96407 (C3H2PO5-), 152.03487 (C7H6NO3-), 223.00121 (C6H8PO7-), 241.01192 (C6H10PO8-), 325.06943 (C11H18PO9-), 601.24054 (C30H37N2O11-)		
ascr	5.99	**556.19574**	78.95779 (PO3-), 96.96849 (H2PO4-)		
	6.15	301.20248	97.06478 (C6H9O-), 99.08043 (C6H11O-), 125.05999 (C7H9O2-), 127.11205 (C8H15O-), 139.11221 (C9H15O-), 143.07082 (C7H11O3-), 157.12311 (C9H17O2-), 201.11310 (C10H17O4-)		
ascr	6.16	**601.24109**	66.03374 (C4H4N-), 67.01775 (C4H3O-), 73.02831 (C3H5O2-), 98.02370 (C4H4NO2-), 108.04457 (C6H6NO-), 134.02412 (C7H4NO2-), 152.03491 (C7H6NO3-), 190.05084 (C10H8NO3-), 203.08264 (C11H11N2O2-), 218.08212 (C12H12NO3-), 234.04044 (C11H8NO5-), 247.11861 (C11H19O6-), 309.12439 (C18H17N2O3-), 335.10370 (C19H15N2O4-), 353.11423 (C19H17N2O5-), 371.12540 (C19H19N2O6-)	603.24109	pasc fragments (see 927.36133 at 4.88 min), 91.05471 (C7H7+), 190.04990 (C10H8NO3+), 218.04485 (C11H8NO4+), 236.05533 (C11H10NO5+), 320.14920 (C17H22NO5+), 355.12878 (C19H19N2O5+), 373.13907 (C19H21N2O6+)
S	6.37	307.12247	96.95601 (HSO4-)		
S	6.50	**337.13315**	96.95601 (HSO4-)		
S	7.09	363.14868	96.95601 (HSO4-)		
	10.53	504.31027	78.95785 (PO3-), 140.01131 (C2H7NPO4-), 196.03786 (C5H11NPO5-), 214.04865 (C5H13NPO6-), 307.26431 (C20H35O2-, major)	506.32443	365.30508 (C23H41O3+)
	11.25	433.23657	78.95785 (PO3-), 96.96835 (H2PO4-), 152.99522 (C3H6PO5-)		
	14.15	423.20795	87.00773 (C3H3O3-), 279.26917 (C19H35O-), 307.26428 (C20H35O2-), 323.25858 (C20H35O3-), 351.25403 (C21H35O4-), 387.23059 (C21H36O4Cl-)		

Table S11. Differential metabolites from *P. pacificus* growth medium, ES- mode, that are decreased or absent in RS2770 *Ppa-daf-22* medium compared to RS2333. Peaks that are present but not differential in J2 medium are shown in blue. Peaks that are also differential inJ2 medium are shown in red. **Peaks that are also in J2 medium table (ES-) are shown in bold red.** Entries that have a corresponding peak in the ES+ table are shaded grey.

class	*smid-db*	*rt (min)*	*m/z (ES-)*	*MS/MS (ES-)*	*m/z (ES+)*	*MS/MS (ES+)*
S		1.12	227.05963			
S		1.96	**211.02846**	see J2, ES- table		
		1.99	229.11926	58.02862 (C2H4NO-), 126.09171 (C7H12NO-), 128.07072 (C6H10NO2-), 141.10266 (C7H13N2O-), 143.11853 (C7H15N2O-), 145.09776 (C6H13N2O2-), 187.10869 (C8H15N2O3-)	231.13370	84.08131 (C5H10N+), 126.09143 (C7H12NO+), 185.12837 (C9H17N2O2+), 189.12326 (C8H17N2O3+), 213.12332 (C10H17N2O3+)
		2.02	970.24817	78.95784 (PO3-), 96.96857 (H2PO4-), 122.98451 (C2H4PO4-), 166.05092 (C8H8NO3-), 168.04283 (C4H11NPO4-), 569.13800 (C20H30N2PO15-), 640.21277 (C24H39N3PO15-), 693.13330 (C29H30N2PO16-), 754.24323 (C29H45N3PO18-), 807.16406 (C34H36N2PO19-), 813.19910 (C37H37N2O19-), 858.25873 (C39H44N3O19-), 872.26892, 911.17596 (C37H40N2PO23-)	972.26267	98.98441 (H4PO4+), 104.10736 (C5H14NO+), 124.99995 (C2H6PO4+), 126.05515 (C6H8NO2+), 184.07324 (C5H15NPO4+), 226.08382 (C7H17NPO5+), 333.12082 (C13H22N2PO6+), 351.13129 (C13H24N2PO7+), 369.14194 (C13H26N2PO8+)
		3.39	414.14084	121.02872 (C7H5O2-), 122.03658 (C7H6O2-, rad), 193.07440 (C10H11NO3-, rad), 208.09798 (C11H14NO3-)		
		3.84	517.16962	78.95773 (PO3-), 96.96838 (H2PO4-), 150.97948 (C3H4PO5-), 223.00137 (C6H8PO7-), 241.01196 (C6H10PO8-)		
ascr	ubas#10	3.94	455.14423	78.95785 (PO3-), 96.96854 (H2PO4-), *102.05505 (C4H8NO2-), 117.05490 (C5H9O3-), *145.06151 (C5H9N2O3-), 163.01643 (C5H8PO4-), 191.01151 (C6H8PO5-), 209.02214 (C6H10PO6-), 309.07483 (C11H18PO8-), 337.08136 (C11H18N2PO8-), 412.13815 (C15H27NPO10-), 438.11728 (C16H25NPO11-); (* fragments present in ubas#3)	457.15817	95.04957 (C6H7O+), 113.05998 (C6H9O2+), 129.06592 (C5H9N2O2+), 193.02597 (C6H10PO5+), 279.06253 (C10H16PO7+), 322.06853 (C11H17NPO8+), 339.09500 (C11H20N2PO8+)
ascr	ubas#11	4.10	573.20709	73.02827 (C3H5O2-), 85.02839 (C4H5O2-), 99.04408 (C5H7O2-), 102.05501 (C4H8NO2-), 127.05063 (C5H7N2O2-), 247.11852 (C11H19O6-), 315.14502 (C15H23O7-), 332.17166 (C15H26NO7-), 375.17752 (C16H27N2O8-)	539.24467	70.06580 (C4H8N+), 84.04493 (C4H6NO+), 86.06055 (C4H8NO+), 104.07093 (C4H10NO2+), 112.03959 (C5H6NO2+), 113.05995 (C6H9O2+), 116.07075 (C5H10NO2+), 129.06586 (C5H9N2O2+), 130.04984 (C5H8NO3+), 147.07637 (C5H11N2O3+), 259.12885 (C11H19N2O5+)
		4.12	609.21942	171.04489 (C11H7O2-), 240.11574 (C16H16O2-, rad), 241.12366 (C16H17O2-), 285.11298 (C17H17O4-), 447.16623 (C23H27O9-)		
		4.26	252.08777	121.02876 (C7H5O2-), 122.03658 (C7H6O2-, rad), 193.07440 (C10H11NO3-, rad), 208.09798 (C11H14NO3-)	254.10216	91.05470 (C7H7+), 95.04956 (C6H7O+), 119.04933 (C8H7O+), 151.07533 (C9H11O2+), 194.08118 (C10H12NO3+), 219.06517 (C12H11O4+), 236.09160 (C12H14NO4+)
ascr	ubas#5	4.33	361.16183	73.02904 (C3H5O2-), 85.02825 (C4H5O2-), 102.05605 (C4H8NO2-), 127.05031 (C5H7N2O2-), 145.06183 (C5H9N2O3-), 158.08220 (C7H12NO3-), 233.10286 (C10H17O6-), 301.12927 (C14H21O7-), 318.15588 (C14H24NO7-)	363.17619	129.06589 (C5H9N2O2+), 147.07635 (C5H11N2O3+), 259.12863 (C11H19N2O5+)
		4.42	379.13763	99.04420 (C5H7O2-), 107.03542 (C3H7O4-), 117.05495 (C5H9O3-), 126.01897	381.15213	56.05032 (C3H6N+), 70.06581 (C4H8N+), 72.08144 (C4H10N+),

				(C5H4NO3-), 134.04663 (C5H4N5-), 160.02623 (C6H2N5O-), 217.08437 (C9H9N6O-), 261.07410 (C10H9N6O3-)		74.06068 (C3H8NO+), *102.05534 (C4H8NO2+), 119.03540 (C5H3N4+), *120.06570 (C4H10NO3+), *136.06178 (C5H6N5+), 137.04575 (C5H5N4O+), *162.04092 (C6H4N5O+), *202.10739 (C9H16NO4+), *220.11790 (C9H18NO5+), *263.08853 (C10H11N6O3+), *281.09912 (C10H13N6O4+); (* fragments present in npar#1 and npar#2)
S		4.55	353.12790	79.95619 (SO3-), 96.95910 (HSO4-), 113.05997 (C6H9O2-), 143.07111 (C7H11O3-), 273.17099 (C14H25O5-)		
		4.70	458.13425	131.03717 (C8H5NO-, rad), 132.04494 (C8H6NO-), 161.04549 (C6H9O5-), 294.09854 (C14H16NO6-)		
		4.74	719.23315			
		4.77	704.22357	78.95788 (PO3-), 130.08678 (C6H12NO2-), 389.10129 (C16H22PO9-), 423.18927 (C17H32N2PO8-)	706.23706	173.05560 (C6H9N2O4+), 230.07729 (C8H12N3O5+)
		4.79	389.10092	78.95785 (PO3-)	391.11542	91.05466 (C7H7+), 149.02330 (C8H5O3+), 165.05452 (C9H9O3+), 179.07013 (C10H11O3+), 197.08081 (C10H13O4+), 212.99461 (C8H6PO5+), 217.02592 (C8H10PO5+), 229.99731 (C8H7PO6+, rad), 231.00507 (C8H8PO6+), 245.02071 (C9H10PO6+), 277.04706 (C10H14PO7+), 345.10950 (C15H22PO7+), 373.10413 (C16H22PO8+)
		4.92	266.10370	58.02866 (C4H4NO-), 121.02874 (C7H5O2-), 136.05241 (C8H8O2-, rad), 168.04274 (C8H8O4-, rad), 222.11372 (C12H16NO3-)	268.11761	91.05470 (C7H7+), 119.04933 (C8H7O+), 151.07538 (C9H11O2+), 165.09100 (C10H13O2+), 194.08116 (C10H12NO3+), 208.09686 (C11H14NO3+), 219.06516 (C12H11O4+), 233.08075 (C13H13O4+), 236.09163 (C12H14NO4+), 250.10718 (C13H16NO4+)
ascr	ubas#12	4.96	389.19366	73.02824 (C3H5O2-), 85.02829 (C4H5O2-), 102.05493 (C4H8NO2-), 113.05978 (C6H9O2-), 127.05044 (C5H7N2O2-), 261.13425 (C12H21O6-), 329.16071 (C16H25O7-), 346.18738 (C16H28NO7-)	391.20749	
ascr		5.03	636.20721	78.95785 (PO3-), 96.96857 (H2PO4-), 148.96414 (C3H2PO5-), 223.00139 (C6H8PO7-), 241.01198 (C6H10PO8-), 275.15018 (C13H23O6-), 192.99060 (C5H6PO6-), 378.05963 (C13H17NPO10-), 499.15906 (C19H32PO13-)	638.22144	97.02882 (C5H5O2+), 98.98457 (H4PO4+), 129.09109 (C7H13O2+), 138.05499 (C7H8NO2+)
		5.10	545.22504	167.03477 (C8H7O4-), 218.09462 (C13H14O3-, rad), 219.06647 (C12H11O4-), 233.11812 (C14H17O3-), 235.09743 (C13H15O4-), 250.12137 (C14H18O4-, rad), 265.14493 (C15H21O4-), 309.13483 (C16H21O6-), 367.13998 (C18H23O8-), 383.17163 (C19H27O8-)	564.26563	127.07548 (C7H11O2+), 151.07542 (C9H11O2+), 154.06247 (C8H10O3+, rad), 169.08589 (C9H13O3+), 182.05743 (C9H10O4+, rad), 197.08090 (C10H13O4+, rad, major), 293.13824 (C16H21O5+), 367.17514 (C19H27O7+)
ascr		5.15	**664.23914**	see 674.26752 in J2, ES- table		
S		5.16	**267.09094**	see 267.09100 in J2, ES- table		
		5.18	423.16635	59.01258 (C2H3O2-), 71.01261 (C3H3O2-), 85.02839 (C4H5O2-), 89.02329 (C3H5O3-), 101.02341 (C4H5O3-), 113.02352 (C5H5O3-), 119.03421 (C4H7O4-), 156.05772 (C11H8O-, rad), 157.06560 (C11H9O-), 197.09715 (C14H13O-), 199.11292 (C14H15O-), 225.09233 (C15H13O2-), 243.10263 (C15H15O3-), 261.11298 (C15H17O4-)	425.18085	

ascr	ubas#13	5.21	803.32336	73.02830 (C3H5O2-), 85.02842 (C4H5O2-), 102.05515 (C4H8NO2-), 127.05055 (C5H7N2O2-), 247.11893 (C11H19O6-), 285.13440 (C14H21O6-), 477.23425 (C22H37O11-), 545.26105 (C26H41O12-), 605.29340 (C27H45N2O13-)	769.36096	101.06001 (C5H9O2+), 113.05988 (C6H9O2+), 129.06583 (C5H9N2O2+), 147.07629 (C5H11N2O3+), 199.09625 (C10H15O4+), 259.12851 (C11H19N2O5+), 341.17047 (C16H25N2O6+), 359.18082 (C16H27N2O7+)
		5.22	**471.18756**	see J2, ES- table		
		5.28	483.22369	83.04906 (C5H7O-), 85.06472 (C5H9O-), 99.08047 (C6H11O-), 179.10767 (C11H15O2-), 197.11826 (C11H17O3-), 241.10812 (C12H17O5-)	485.23981	119.08573 (C9H11+), 147.08037 (C10H11O+), 161.09604 (C11H13O+), 189.09091 (C12H13O2+), 207.10167 (C12H15O3+), 225.11211 (C12H17O4+), 243.12257 (C12H19O5+)
		5.33	764.26575	78.95795 (PO3-), 96.96865 (H2PO4-), 148.96419 (C3H2PO5-), 223.00151 (C6H8PO7-), 291.02783 (C10H12PO8-), 309.03806 (C10H14PO9-), 326.06540 (CC10H17NPO9-), 334.03305 (C11H13NPO9-), 351.05954 (C11H16N2PO9-), 352.04382 (C11H15NPO10-), 506.11871 (C18H25N3PO12-), 610.19141 (C24H37NPO15-), 627.21753 (C24H40N2PO15-), 721.25708 (C30H46N2PO16-), 747.23853 (C31H44N2PO17-)	766.28025	108.04473 (C6H6NO+), 109.02869 (C6H5O2+), 127.03907 (C6H7O3+), 129.06590 (C5H9N2O2+), 130.04994 (C5H8NO3+), 147.07629 (C5H11N2O3+), 189.08693 (C7H13N2O4+), 225.01579 (C6H10PO7+), 237.08665 (C11H13N2O4+), 238.07079 (C11H12NO5+), 255.09726 (C11H15N2O5+), 273.10785 (C11H17N2O6+), 353.07352, 371.08475, 383.18121 (C18H27N2O7+), 401.1903 (C18H29N2O8+), 499.16748 (C18H32N2PO12+)
		5.40	227.12906	85.06476 (C5H9O-), 115.07565 (C6H11O2-), 129.09145 (C7H13O2-), 135.11729 (C10H15-), 147.011743 (C11H15-), 181.12355 (C11H17O2-), 183.13904 (C11H19O2-)	229.14356	
		5.41	**215.12904**	see J2, ES- table		
ascr	ubas#14	5.42	827.36823	73.02822 (C3H5O2-), 85.02835 (C4H5O2-), 619.30884 (C28H47N2O13-)	783.37640	69.07053 (C5H9+), 113.05991 (C6H9O2+), 115.07555 (C6H11O2+), 129.06584 (C5H9N2O2+), 147.07631 (C5H11N2O3+), 259.12854 (C11H19N2O5+), 355.18628 (C17H27N2O6+), 373.19672 (C17H29N2O7+)
		5.53	760.27118	78.95785 (PO3-), 96.96856 (H2PO4-), 148.96408 (C3H2PO5-), 207.00677 (C6H8PO6-), 293.04361 (C10H14PO8-), 310.06946 (C10H17NPO8-), 336.04984 (C11H15NPO9-), 353.07584 (C11H18N2PO9-), 356.05450 (C14H15NPO8-), 424.08057 (C18H19NPO9-), 442.09070 (C18H21NPO10-), 459.11758 (C18H24N2PO10-), 485.09708 (C19H22N2PO11-), 502.12344 (C19H25N3PO11-), 717.26654 (C31H46N2PO15-), 743.24451 (C32H44N2PO16-)	762.28568	same fragments as for 766.28025 at 5.33 min
		5.55	591.27740	see comments	see growth medium, ES+ table	
		5.71	449.18237	59.01258 (C2H3O2-), 71.01263 (C3H3O2-), 85.02843 (C4H5O2-), 89.02339 (C3H5O3-), 101.02351 (C4H5O3-), 113.02367 (C5H5O3-), 119.03421 (C4H7O4-), 156.05772 (C11H8O-, rad), 188.04774 (C11H8O3-, rad), 225.12859 (C16H17O-), 243.13911 (C16H19O2-)	451.19687, 468.22339	157.06483 (C11H9O+), 253.12219 (C17H17O2+), 271.13269 (C17H19O3+)
ascr		5.92	505.26627	73.02837 (C3H5O2-), 127.07578 (C7H11O2-), 275.14993 (C13H23O6-)	524.30750	213.11208 (C11H17O4+), 231.12259 (C11H19O5+), 243.12248 (C12H19O5+)
ascr		5.94	**556.19598**	see J2, ES- table	558.21048	202.08620 (C12H12NO2+)

ascr		5.97	727.21350	73.02828 (C3H5O2-), 78.95789 (PO3-), 92.04963 (C6H6N-), 96.96871 (H2PO4-), 136.03992 (C7H6NO2-), 148.96420 (C3H2PO5-), 162.97992 (C4H4PO5-), 453.11658 (C17H26PO12-), 590.16559 (C24H33NPO14-)	729.22800	92.05000 (C6H6N+), 101.06001 (C5H9O2+), 120.04459 (C7H6NO+), 127.03911 (C6H7O3+), 132.04424 (C8H6NO+), 138.05495 (C7H8NO2+), 204.06557 (C11H10NO3+), 209.08099 (C11H13O4+), 216.06531 (C12H10NO3+), 225.01575 (C6H10PO7+), 228.06548 (C13H10NO3+), 246.07602 (C13H12NO4+), 264.08643 (C13H14NO5+), 362.06335 (C13H17NPO9+)
		6.04	431.14777	78.95784 (PO3-)	433.16227	151.07535 (C9H11O2+), 179.07019 (C10H11O3+), 245.02086 (C9H10PO6+), 277.04694 (C10H14PO7+), 317.07819 (C13H18PO7+)
ascr		6.18	**601.24078**	see J2, ES- table		
ascr		6.18	894.35376	78.95786 (PO3-), 96.96860 (H2PO4-), 127.07582 (C7H11O2-), 136.03992 (C7H6NO2-), 148.96420 (C3H2PO5-), 192.99057 (C5H6PO6-), 223.00151 (C6H8PO7-), 241.01205 (C6H10PO8-), 275.15070 (C13H23O6-), 378.06049 (C13H17NPO10-), 757.30591 (C32H54PO18-)	896.36826	97.02883 (C5H5O2+), 98.98456 (H4PO4+), 111.08075 (C7H11O+), 113.06001 (C6H9O2+), 120.04455 (C7H6NO+), 127.03911 (C6H7O3+), 129.09109 (C7H13O2+), 138.05490 (C7H8NO2+), 145.04947 (C6H9O4+), 225.01576 (C6H10PO7+), 232.09660 (C13H14NO3+), 241.14326 (C13H21O4+), 243.02629 (C6H12PO8+), 250.10779 (C13H16NO4+), 255.12302 (C13H19O5+), 259.15393 (C13H23O5+), 268.11813 (C13H18NO5+), 353.09933 (C13H22PO9+), 371.11011 (C13H24PO10+), 378.19138 (C20H28NO6+)
S		6.35	**337.13330**	see J2, ES- table		
ascr		6.51	755.24402	78.95787 (PO3-), 92.04950 (C6H6N-), 96.96857 (H2PO4-), 136.03987 (C7H6NO2-), 148.96422 (C3H2PO5-), 223.00208 (C6H8PO7-), 342.03897 (C13H13NPO8-), 618.19501 (C26H37NPO14-)	757.25852	120.04461 (C7H6NO+, major), 138.05502 (C7H8NO2+), 246.07587 (C13H12NO4+), 264.08636 (C13H14NO5+), 362.06323 (C13H17NPO9+)
		6.63	256.15564	74.02354 (C2H4NO2-), 194.15512 (12H20NO-)	240.15952	76.03992 (C2H6NO2+), 194.15396 (C12H20NO+)
		6.67	670.19171	78.95782 (PO3-), 96.96854 (H2PO4-), 204.99052 (C6H6PO6-),223.00117 (C6H8PO7-), 241.01195 (C6H10PO8-), 515.13336 (C22H28PO12-), 533.14276 (C22H30PO13-)	672.20621	120.04471 (C7H6NO+), 127.03910 (C6H7O3+), 151.07544 (C9H11O2+), 154.06230 (C8H10O3+, rad), 169.08574 (C9H13O3+), 182.05737 (C9H10O4+, rad), 197.08089 (C10H13O4+, major), 293.13837 (C16H21O5+), 309.13306 (C16H21O6+)
ascr	tasc#1	7.65	791.44427	73.02825 (C3H5O2-), 127.07572 (C7H11O2-), 145.08659 (C7H13O3-), 275.14987 (C13H23O6-), 533.29700 (C26H45O11-)	793.45877, 810.48486	83.08608 (C6H11+), 85.06532 (C5H9O+), 95.04955 (C6H7O+), 111.08073 (C7H11O+), 113.05994 (C6H9O2+), 129.09105 (C7H13O2+), 147.10156 (C7H15O3+), 183.13792 (C11H19O2+), 207.10165 (C12H15O3+), 225.11206 (C12H17O4+), 241.14323 (C13H21O4+), 259.15381 (C13H23O5+), 353.19553 (C19H29O6+), 371.20633 (C19H31O7+), 389.21716 (C19H33O8+)
		7.72	449.27560		422.31140, 427.26642	
ascr		8.21	567.28156	73.02827 (C3H5O2-), 127.07578 (C7H11O2-), 151.03975 (C8H7O3-), 165.05545 (C9H9O3-), 166.02692 (C8H6O4-, rad), 167.03485 (C8H7O4-), 181.05081 (C9H9O4-), 275.14999	586.32312, 591.27826	113.06007 (C6H9O2+), 127.07548 (C7H11O2+), 136.05191 (C8H8O2+, rad), 137.05974 (C8H9O2+), 151.07542 (C9H11O2+), 154.06244 (C8H10O3+, rad), 169.08583

				(C13H23O6-), 535.25507 (C28H39O10-)		(C9H13O3+), 182.05743 (C9H10O4+, rad), 197.08086 (C10H13O4+, major), 261.11240 (C15H17O4+), 293.13837 (C16H21O5+)
		8.24	371.97586		213.14853	
		10.03	355.15863			

Table S12. Differential metabolites from *P. pacificus* J2 medium, ES+ mode, that are decreased or absent in RS2770 *Ppa-daf-22* medium compared to RS2333. Peaks that are present but not differential in growth medium are shown in blue. Peaks that are also differential in growth medium are shown in red. **Peaks that are also in growth medium table (ES+) are shown in bold red.** Entries that have a corresponding peak in the ES- table are shaded grey.

class	*smid-db*	*rt (min)*	*m/z (ES+)*	*MS/MS (ES+)*	*m/z (ES-)*
		1.00	419.14795	91.05475 (C7H7+), 119.04942 (C8H7O+), 123.04424 (C7H7O2+), 130.04985 (C5H8NO3+), 136.07576 (C8H10NO+), 147.04416 (C9H7O2+), 162.02190 (C5H8NSO3+), 165.05464 (C9H9O3+), 182.08116 (C9H12NO3+), 238.07434 (C8H16NSO5+)	
		1.02	466.30219	58.06596 (C3H8N+), 84.08135 (C5H10N+), 98.09685 (C6H12N+), 116.10728 (C6H14NO+), 126.09153 (C7H12NO+), 128.10715 (C7H14NO+), 144.10172 (C7H14NO2+), 150.09152 (C9H12NO+), 240.17059 (C12H22N3O2+), 351.23886 (C18H31N4O3+), 369.24954 (C18H33N4O4+)	
ascr		2.96	316.21198	70.06584 (C4H8N+), 99.08086 (C6H11O+), 116.07085 (C5H10NO2+), 126.09153 (C7H12NO+), 186.14885 (C10H20NO2+), 200.12817 (C10H18NO3+)	
ascr		3.14	433.16763	see J2, ES- table	
S		3.38	306.10083	see J2, ES- table	
ascr		3.78	586.23486	see J2, ES- table	
		3.97	223.09423		
		4.07	285.13086		
		4.67	583.20569	105.07027 (C8H9+), 121.06500 (C8H9O+), 204.10207 (C12H14NO2+); 5.0 min peak additionally has 120.04470 (C7H6NO+)	
		4.71	734.23242	105.07027 (C8H9+), 136.03941 (C7H6NO2+), 204.10210 (C12H14NO2+), 222.11243 (C12H16NO3+), 244.06050 (C13H10NO4+), 264.12289 (C14H18NO4+), 330.13348 (C18H20NO5+)	
ascr		4.87	927.36133	see J2, ES- table	
		5.04	718.23773	see J2, ES- table	
ascr		5.15	562.20532	see J2, ES- table	
ascr		5.15	**647.30286**	see J2, ES- table	
		5.21	733.30493	97.02882 (C5H5O2+), 120.08099 (C8H10N+), 135.03032 (C5H3N4O+), 152.05673 (C5H6N5O+), 153.04076 (C5H5N4O2+), 202.08643 (C12H12NO2+), 220.09691 (C12H14NO3+), 316.11813 (C17H18NO5+), 334.12839 (C17H20NO6+), 452.19226 (C23H26N5O5+), 485.17850 (C22H25N6O7+), 503.18915 (C22H27N6O8+), 603.24066 (C27H35N6O10+)	
		5.22	**490.22897**	see J2, ES- table	
		5.26	529.24115	164.09314 (C7H10N5+)	
ascr		5.27	476.18973	127.03675 (C4H8O3Na+), 184.07330 (C10H11NONa+), 242.07794 (C12H13NO3Na+), 257.09930 (C10H18O6Na+)	452.19333
ascr		5.39	661.31818	see J2, ES- table	
ascr		5.39	564.24164	141.05228 (C5H10O3Na+), 184.07339 (C10H11NONa+), 271.11508 (C11H20O6Na+), 316.11563 (C15H19NO5Na+)	
ascr		5.42	**765.30865**	see J2, ES- table	
		5.44	747.32025	97.02882 (C5H5O2+), 120.08099 (C8H10N+), 135.03032 (C5H3N4O+), 152.05673 (C5H6N5O+), 153.04076 (C5H5N4O2+), 202.08643 (C12H12NO2+), 220.09691 (C12H14NO3+), 316.11813 (C17H18NO5+), 334.12839 (C17H20NO6+), 466.20773 (C24H28N5O5+), 485.17850 (C22H25N6O7+), 617.25757 (C28H37N6O10+)	
		5.65	519.19788	101.02374 (C4H5O3+), 103.05464 (C8H7+), 120.08102 (C8H10N+), 146.06009 (C9H8NO+), 156.08087 (C11H10N+), 157.06494 (C11H9O+), 174.09135 (C11H12NO+), 184.07565 (C12H10NO+), 202.08633 (C12H12NO2+), 220.09686 (C12H14NO3+), 228.06552 (C13H10NO3+), 238.10753 (C12H16NO4+), 262.10718 (C14H16NO4+), 346.12881 (C18H20NO6+), 364.13895 (C18H22NO7+), 382.14972 (C18H24NO8+)	
ascr		5.71	544.19452	see J2, ES- table	
ascr		5.76	749.31293	see J2, ES- table	
ascr		6.16	603.25531	see J2, ES- table	
		6.31	730.31995	99.08089 (C6H11O+), 109.02870 (C6H5O2+), 127.03911 (C6H7O3+), 136.07596 (C8H10NO+), 145.04970 (C6H9O4+), 177.12747 (C12H17O+), 184.07324 (C5H15NPO4+)), 195.13792 (C12H19O2+), 225.01587 (C6H10PO7+), 267.12320 (C14H19O5+), 321.16983 (C18H25O5+), 339.17993 (C18H27O6+)	728.30527
		6.45	525.18475	244.09453 (C12H15NO3Na+), 388.13678 (C18H23NO7Na+)	
ascr		6.57	481.25488	101.02374 (C4H5O3+), 103.05464 (C8H7+), 120.08102 (C8H10N+), 146.06009	

				(C9H8NO+), 156.08087 (C11H10N+), 157.06494 (C11H9O+), 174.09135 (C11H12NO+), 184.07565 (C12H10NO+), 202.08633 (C12H12NO2+), 220.09686 (C12H14NO3+), 238.10753 (C12H16NO4+)	
		7.00	639.25244	141.05228 (C5H10O3Na+), 184.07372 (C10H11NONa+), 190.04985 (C10H8NO3+), 202.08633 (C12H12NO2+), 391.12634 (C20H20N2O5Na+)	615.25593
		7.17	569.24957	see comments	
		7.29	**309.13324**	171.08043 (C12H11O+), 195.10165 (C11H15O3+), 197.08070 (C10H13O4+), 199.07539 (C13H11O2+), 217.08594 (C13H13O3+), 231.10165 (C14H15O3+), 259.09628 (C15H15O4+), 263.12775 (C15H19O4+), 291.12262 (C16H19O5+)	see growth medium, ES+ table
		7.50	601.27594	55.01865 (C3H3O+), 91.05473 (C7H7+), 103.05456 (C8H7+), 120.08099 (C8H10N+), 146.06017 (C9H8NO+), 156.08092 (C11H10N+), 157.06480 (C11H9O+), 174.09132 (C11H12NO+), 184.07574 (C12H10NO+), 202.08633 (C12H12NO2+), 220.09682 (C12H14NO3+), 234.07614 (C12H12NO4+), 320.14926 (C17H22NO5+), 353.14954 (C20H21N2O4+)	
		8.04	255.23172	219.21065 (C16H27+), 237.22112 (C16H29O+)	
		8.22	675.37836	56.96563 (CaOH+), 115.00687 (C3H7O2Ca+), 171.06929 (C7H15O2Ca+), 189.07980 (C7H17O3Ca+), 251.09470 (C12H19O3Ca+), 269.10602 (C12H21O4Ca+), 287.11633 (C12H23O5Ca+), 463.23657 (C24H39O6Ca+), 481.24756 (C24H41O7Ca+)	
		10.52	506.32443	see J2, ES- table	

Table S13. Differential metabolites from *P. pacificus* growth medium, ES+ mode, that are decreased or absent in RS2770 *Ppa-daf-22* medium compared to RS2333. Peaks that are present but not differential in J2 medium are shown in blue. Peaks that are also differential in J2 medium are shown in red. **Peaks that are also in J2 medium table (ES+) are shown in bold red.** Entries that have a corresponding peak in the ES- table are shaded grey.

class	*smid-db*	*rt (min)*	*m/z (ES+)*	*MS/MS (ES+)*	*m/z (ES-)*	*MS/MS (ES-)*
		2.00	231.13370	see growth medium, ES- table		
		4.30	695.25238	152.05669 (C5H6N5O+), 165.09102 (C10H13O2+), 208.09702 (C11H14NO3+), 284.09857 (C10H14N5O5+), 563.21045 (C24H31N6O10+)		
		4.34	254.10216	see growth medium, ES- table		
		4.58	428.16656	129.06589 (C5H9N2O2+), 147.07639 (C5H11N2O3+), 153.01814 (C7H5O4+), 220.09682 (C12H14NO3+), 228.06551 (C13H10NO3+), 238.07086 (C11H12NO5+), 253.06729 (C7H13N2O8+), 256.08136 (C11H14NO6+), 266.13834 (C14H20NO4+), 273.10806 (C11H17N2O6+), 291.11847 (C11H19N2O7+)	462.12891, 472.15744	92.04958 (C6H6N-), 127.05065 (C5H7N2O2-), 136.03986 (C7H6NO2-)
		4.75	706.23706	see growth medium, ES- table		
		4.77	391.11456	91.05470 (C7H7+), 151.07533 (C9H11O2+), 165.05464 (C9H9O3+), 179.07021 (C10H11O3+), 197.08083 (C10H13O4+), 245.02080 (C14H6O3Na+), 277.04700 (C15H10O4Na+), 345.10962 (C20H18O4Na+), 373.10434 (C21H18O5Na+)		
ascr	ubas#8	4.78	497.22470	66.03432 (C4H4N+), 93.04485 (C5H5N2+), 121.03969 (C6H5N2O+), 129.06584 (C5H9N2O2+), 319.12891 (C16H19N2O5+), 379.16119 (C17H23N4O6+)	495.20965	73.02824 (C3H5O2-), 85.02834 (C4H5O2-), 93.04472 (C5H5N2-), 102.05504 (C4H8NO2-), 119.02426 (C6H3N2O-), 137.03505 (C6H5N2O2-), 367.15103 (C17H23N2O7-), 435.17740 (C21H27N2O8-), 452.20419 (C21H30N3O8-), 478.18317 (C22H28N3O9-)
		4.91	268.11761	see growth medium, ES- table		
		4.96	435.20654	104.05318 (C4H10NS+), 110.09667 (C7H12N+), *118.06528 (C8H8N+), 120.08090 (C8H10N+), 127.08659 (C6H11N2O+), 129.10228 (C6H13N2O+), *132.08075 (C9H10N+), *146.06000 (C9H8NO+), 158.09978 (C8H16NS+), *159.09158 (C10H11N2+), *188.07047 (C11H10NO2+), 203.12114 (C9H19N2SO+), *205.09706 (C11H13N2O2+), 231.11601 (C10H19N2SO2+), 304.16534 (C16H22N3O3+); (* Trp fragments)	433.19204	*74.02349 (C2H4NO2-), 99.05527 (C4H7N2O-), 115.08682 (C5H11N2O-), *116.04970 (C8H6N-), 129.10262 (C6H13N2O-), *142.06570 (C10H8N-), *159.09250 (C10H11N2-), 164.07141 (C9H10NO2-), 198.12485 (C9H16N3O2-), *203.08264 (C11H11N2O2-), 229.10146 (C10H17N2SO2-), 304.13373 (C12H22N3SO4-); (* Trp fragments)
ascr		5.02	638.22144	see growth medium, ES- table		
		5.08	564.26563	see growth medium, ES- table		
ascr	npar#4	5.09	689.24530	102.05534 (C4H8NO2+), 120.06574 (C4H10NO3+), 134.04614 (C5H4N5+), 152.05676 (C5H6N5O+), 160.02501 (C6H2N5O+), 165.02298 (C6H5N4S+), 182.04947 (C6H8N5S+), 202.10747 (C9H16NO4+), 208.02882 (C7H6N5SO+), 220.11800 (C9H18NO5+), 309.07666 (C11H13N6SO3+), 327.08682 (C11H15N6SO4+), 340.07095 (C12H14N5SO5+), 427.13959 (C16H23N6SO6+)	687.23080	73.02824 (C3H5O2-), 99.04413 (C5H7O2-), 111.04429 (C6H7O2-), 126.01894 (CC5H4NO3-), 147.06561 (C6H11O4-), 180.03470 (C6H6N5S-), 247.11861 (C11H19O6-), 286.12991 (C13H20NO6-), 348.16632 (C15H26NO8-), 374.14569 (C16H24NO9-)
ascr		5.15	**647.30292**	see 674.26752 in J2, ES- table		
		5.18	488.21335	143.08553 (C11H11+), 171.08041 (C12H11O+), 189.09097 (C12H13O2+), 199.07541 (C13H11O2+), 217.08595	469.17154	217.05052 (C12H9O4-), 232.07396 (C13H12O4-, rad), 247.09740 (C14H15O4-),

				(C13H13O3+), 227.07021 (C14H11O3+), 231.10155 (C14H15O3+), 259.09650 (C15H15O4+), 277.10712 (C15H17O5+), 291.12250 (C16H19O5+), 309.13318 (C16H21O6+)		262.12082 (C15H18O4-, rad), 263.12869 (C15H19O4-), 425.18182 (C21H29O9-)
ascr	ubas#13	5.21	769.36096	see growth medium, ES- table		
		5.22	**490.22900**	see 471.18762 (-) in J2, ES- table		
		5.26	485.23981	see growth medium, ES- table		
ascr	ubas#15	5.36	550.24176	55.01870 (C3H3O+), 102.03761 (C4H8NS+), 113.05998 (C6H9O2+), 115.02142 (C5H7SO+), 129.06592 (C5H9N2O2+), 132.04782 (C5H10NSO+), 139.07536 (C8H11O2+), 167.07008 (C9H11O3+), 174.05838 (C7H12NSO2+), 185.08066 (C9H13O4+), 192.06866 (C7H14NSO3+), 241.10699 (C12H17O5+), 253.10693 (C13H17O5+), 296.11270 (C14H18NO6+), 313.13928 (C14H21N2O6+), 372.14728 (C17H26NSO6+), 389.17410 (C17H29N2SO6+), 415.15356 (C18H27N2SO7+), 432.17987 (C18H30N3SO7+)	548.22834	58.02841 (C2H4NO-), 71.01244 (C3H3O2-), 85.02815 (C4H5O2-), 99.04399 (C5H7O2-), 102.05476 (C4H8NO2-), 118.03209 (C4H8NSO-), 127.05003 (C5H7N2O2-), 301.12866 (C14H21O7-), 369.15445 (C18H25O8-), 429.18689 (C19H29N2O9-)
		5.37	723.36334	141.02232 (C5H9O2Ca+), 155.03784 (C6H11O2Ca+), 173.04855 (C6H13O3Ca+), 187.06413 (C7H15O3Ca+), 199.06429 (C8H15O3Ca+), 205.07477 (C7H17O4Ca+), 223.10034 (C11H19O2Ca+), 241.11084 (C11H21O3Ca+), 267.09009 (C12H19O4Ca+), 285.10077 (C12H21O5Ca+), 495.22684 (C24H39O8Ca+)	see 227.12906 in growth medium, ES- table	
ascr	ubas#14	5.42	783.37640	see growth medium, ES- table		
ascr		5.43	**782.33484**	see 763.29425 in J2, ES- table		
		5.53	282.13367	91.05473 (C7H7+), 103.05461 (C8H7+), 105.07026 (C8H9+), 107.04955 (C7H7O+), 119.04937 (C8H7O+), 133.06487 (C9H9O+), 150.06757 (C9H10O2+, rad), 151.07545 (C9H11O2+), 165.09102 (C10H13O2+), 194.08138 (C10H12NO3+), 208.09688 (C11H14NO3+), 233.08095 (C13H13O4+)		
ascr		5.55	728.33911	101.02374 (C4H5O3+), 103.05464 (C8H7+), 120.08102 (C8H10N+), 144.08086 (C10H10N+), 146.06009 (C9H8NO+), 156.08087 (C11H10N+), 157.06494 (C11H9O+), 174.09135 (C11H12NO+), 184.07565 (C12H10NO+), 202.08633 (C12H12NO2+), 220.09686 (C12H14NO3+), 238.10753 (C12H16NO4+), 261.12311 (C14H17N2O3+)	726.32461	
ascr		5.55	593.29175	83.04973 (C5H7O+), 87.04459 (C4H7O2+), 113.06001 (C6H9O2+), 129.06593 (C5H9N2O2+), 130.04999 (C5H8NO3+), 147.07642 (C5H11N2O3+), 199.09677 (C10H15O4+), 259.12875 (C11H19N2O5+), 327.15491 (C15H23N2O6+), 345.16559 (C15H25N2O7+)	see growth medium, ES- table	
		5.94	275.13922	118.06543 (C8H8N+), 130.06519 (C9H8N+), 132.08092 (C9H10N+), 146.06007 (C9H8NO+), 159.09166 (C10H11N2+), 188.07060 (C11H10NO2+), 205.09732 (C11H13N2O2+), 229.13359 (C14H17N2O+)	273.12472	*74.02348 (C2H4NO2-), 86.05991 (C4H8NO-), *116.04958 (C8H6N-), 144.06598 (C6H10NO3-), *159.09238 (C10H11N2-), *203.08261 (C11H11N2O2-); (* Trp fragments)
ascr	ubas#16, 17	6.05	596.28204	ubas#16: 101.02375 (C4H5O3+), 103.05464 (C8H7+), 104.07110 (C4H10NO2+), 113.05990 (C6H9O2+), 120.08096 (C8H10N+), 129.06593 (C5H9N2O2+), 147.07635 (C5H11N2O3+), 174.09108 (C11H12NO+), 202.08604 (C12H12NO3+), 220.09677 (C12H14NO3+), 259.12839 (C11H19N2O5+); ubas#17: 91.05474 (C7H7+), 03.05466 (C8H7+), 113.06017	594.26683	73.02805 (C3H5O2-), 85.02814 (C4H5O2-), 98.02347 (C4H4NO2-), 102.05483 (C4H8NO2-), 127.05022 (C5H7N2O2-), 218.08160 (C12H12NO3-), 247.11832 (C11H19O6-), 315.14447 (C15H23O7-), 332.17105 (C15H26NO7-), 375.17661 (C16H27N2O8-)

				(C6H9O2+), 120.08099 (C8H10N+), 129.06592 (C5H9N2O2+), 146.06006 (C9H8NO+), 156.08089 (C11H10N+), 174.09140 (C11H12NO+), 184.07570 (C12H10NO+), 202.08604 (C12H12NO3+), 220.09677 (C12H14NO3+), 400.17554 (C22H26NO6+), 417.20193 (C22H29N2O6+), 435.21286 (C22H31N2O7+), 460.20792 (C23H30N3O7+), 478.21890 (C23H32N3O8+)		
		6.06	297.18112	87.05581 (C3H7N2O+), 88.03981 (C3H6NO2+), 116.03448 (C4H6NO3+), 133.06082 (C4H9N2O3+), 150.12778 (C10H16N+), 165.12738 (C11H17O+), 182.15417 (C11H20NO+), 192.13829 (C12H18NO+), 234.14865 (C14H20NO2+), 251.17503 (C14H23N2O2+), 252.15918 (C14H22NO3+), 280.15421 (C15H22NO4+)		
ascr	ubas#18	6.11	626.29272	91.05470 (C7H7+), 119.04939 (C8H7O+), 129.06592 (C5H9N2O2+), 151.07530 (C9H11O2+), 250.10721 (C13H16NO4+), 268.11761 (C13H18NO5+), 448.19656 (C23H30NO8+), 465.22342 (C23H33N2O8+), 491.20313 (C24H31N2O9+), 508.22946 (C24H34N3O9+)	624.27740	73.02808 (C3H5O2-), 85.02812 (C4H5O2-), 98.02361 (C4H4NO2-), 99.04397 (C5H7O2-), 102.05483 (C4H8NO2-), 127.05057 (C5H7N2O2-), 233.06892 (C9H13O7- ?), 247.11806 (C11H19O6-), 248.09222 (C13H14NO4-), 315.14420 (C15H23O7-), 332.17181 (C15H26NO7-), 375.17618 (C16H27N2O8-)
ascr		6.11	720.34467	151.07533 (C9H11O2+), 154.06245 (C8H10O3+, rad), 169.08585 (C9H13O3+), 182.05714 (C9H10O4+, rad), 197.08086 (C10H13O4+), 293.13824 (C16H21O5+)	701.30417	73.02823 (C3H5O2-), 111.04420 (C6H7O2-), 139.03940 (C7H7O3-), 150.03181 (C8H6O3-, rad), 151.03979 (C8H7O3-), 165.05540 (C9H9O3-), 166.02684 (C8H6O4-, rad), 167.03468 (C8H7O4-), 168.04256 (C8H8O4-, rad), 172.05261 (C11H8O2-, rad), 181.05052 (C9H9O4-), 185.06055 (C12H9O2-), 195.06606 (C10H11O4-), 218.09492 (C13H14O3-, rad), 235.09763 (C13H15O4-), 247.11876 (C11H19O6-), 250.12074 (C14H18O4-, rad), 277.10776 (C15H17O5-), 291.12466 (C16H19O5-), 309.13461 (C16H21O6-), 339.16058 (C21H23O4-), 501.21332 (C27H33O9-), 539.24957 (C27H39O11-)
ascr		6.13	896.36810	97.02884 (C5H5O2+), 98.98459 (H4PO4+), 111.08079 (C7H11O+), 113.06005 (C6H9O2+), 127.03905 (C6H7O3+), 129.09106 (C7H13O2+), 138.05504 (C7H8NO2+), 145.04953 (C6H9O4+), 225.01570 (C6H10PO7+), 232.09660 (C13H14NO3+), 241.14357 (C13H21O4+), 243.02361 (C6H12PO8+), 259.15414 (C13H23O5+), 353.09943 (C13H22PO9+), 371.10974 (C13H24PO10+)	894.35360	73.02827 (C3H5O2-), 78.95783 (PO3-), 92.04933 (C6H6N-), 96.96856 (H2PO4-), 127.07549 (C7H11O2-), 136.03966 (C7H6NO2-), 148.96407 (C3H2PO5-), 150.97972 (C3H4PO5-), 162.97954 (C4H4PO5-), 192.99068 (C5H6PO6-), 223.00137 (C6H8PO7-), 241.01195 (C6H10PO8-), 275.15009 (C13H23O6-), 378.05991 (C13H17NPO10-), 757.30573 (C32H54PO18-)
ascr		6.15	538.32269	111.08077 (C7H11O+), 113.06001 (C6H9O2+), 129.09111 (C7H13O2+), 147.10173 (C7H15O3+), 183.13802 (C11H19O2+), 225.11232 (C12H17O4+), 241.14336 (C13H21O4+), 259.15393 (C13H23O5+)	519.28219	73.02824 (C3H5O2-), 113.05991 (C6H9O2-), 127.07569 (C7H11O2-), 261.13422 (C12H21O6-), 275.14981 (C13H23O6-)
ascr	ubas#19	6.36	315.15500	57.03430 (C3H5O+), 69.03418 (C4H5O+), 95.04958 (C6H7O+), 113.05995 (C6H9O2+),	431.20350	59.02386 (CH3N2O-), 73.02825 (C3H5O2-), 85.02833 (C4H5O2-),

				129.06590 (C5H9N2O2+), 141.09082 (C8H13O2+), 169.08582 (C9H13O3+), 255.12251 (C13H19O5+), 259.12848 (C11H19N2O5+), 298.12836 (C14H20NO6+), 315.15491 (C14H23N2O6+)		99.04417 (C5H7O2-), 102.05508 (C4H8NO2-), 127.05061 (C5H7N2O2-), 129.05496 (C6H9O3-), 145.06137 (C5H9N2O3-), 303.14502 (C14H23O7-), 371.17090 (C18H27O8-), 388.19791 (C18H30NO8-)
ascr	ubas#20	6.53	826.39734	100.03970 (C4H6NO2+), 103.05465 (C8H7+), 113.05997, (C6H9O2+), 120.08103 (C8H10N+), 129.06590 (C5H9N2O2+), 146.06020 (C9H8NO+), 156.08092 (C11H10N+), 157.06482 (C11H9O+), 174.09148 (C11H12NO+), 184.07574 (C12H10NO+), 202.08629 (C12H12NO2+), 220.09645 (C12H14NO3+), 400.17545 (C22H26NO6+), 417.20221 (C22H29N2O6+), 460.20792 (C23H30N3O7+), 478.21887 (C23H32N3O8+), 578.27087 (C28H40N3O10+)	824.38226	73.02824 (C3H5O2-), 85.02833 (C4H5O2-), 98.02370, (C4H4NO2-), 102.05502 (C4H8NO2-), 127.05061 (C5H7N2O2-), 218.08199 (C12H12NO3-), 247.11868 (C11H19O6-), 315.14481 (C15H23O7-), 375.17725 (C16H27N2O8-)
ascr	pasy#12	6.56	481.25507	91.05465 (C7H7+), 103.05454 (C8H7+), 113.05994 (C6H9O2+), 120.08092 (C8H10N+), 146.05998 (C9H8NO+), 156.08080 (C11H10N+), 174.09129 (C11H12NO+), 184.07564 (C12H10NO+), 202.08618 (C12H12NO2+, major)		
ascr	ubas#21	6.58	649.35498	104.07088 (C4H10NO2+), 112.03951 (C5H6NO2+), 113.06001 (C6H9O2+), 115.07561 (C6H11O2+), 129.06590 (C5H9N2O2+), 130.04994 (C5H8NO3+), 147.07639 (C5H11N2O3+), 199.09647 (C10H15O4+), 242.10191 (C11H16NO5+), 259.12869 (C11H19N2O5+), 295.15359 (C16H23O5+), 355.18622 (C17H27N2O6+), 373.19687 (C17H29N2O7+)	647.33966	73.02824 (C3H5O2-), 85.02834 (C4H5O2-), 102.05501 (C4H8NO2-), 113.05993 (C6H9O3-), 127.07570 (C7H11O2-), 257.13962 (C13H21O5-), 261.13425 (C12H21O6-), 275.14978 (C13H23O6-), 343.17657 (C17H27O7-), 519.28101 (C25H43O11-), 587.30743 (C29H47O12-)
		6.59	748.37567	151.07533 (C9H11O2+), 154.06238 (C8H10O3+, rad), 169.08585 (C9H13O3+), 182.05730 (C9H10O4+, rad), 197.08081 (C10H13O4+, major), 293.13815 (C16H21O5+)	729.33517	73.02823 (C3H5O2-), 111.04420 (C6H7O2-), 127.07570 (C7H11O2-), 139.03940 (C7H7O3-), 150.03181 (C8H6O3-, rad), 151.03979 (C8H7O3-), 165.05540 (C9H9O3-), 166.02684 (C8H6O4-, rad), 167.03468 (C8H7O4-), 168.04256 (C8H8O4-, rad), 172.05261 (C11H8O2-, rad), 181.05052 (C9H9O4-), 195.06606 (C10H11O4-), 218.09492 (C13H14O3-, rad), 250.12074 (C14H18O4-, rad), 275.14993 (C13H23O6-), 277.10776 (C15H17O5-), 291.12466 (C16H19O5-), 309.13461 (C16H21O6-), 501.21332 (C27H33O9-), 567.28113 (C29H43O11-)
		6.64	240.15952	see growth medium, ES- table		
		6.64	689.29254	92.04993 (C6H6N+), 111.08071 (C7H11O+), 120.04457 (C7H6NO+), 127.03905 (C6H7O3+), 129.09109 (C7H13O2+), 132.04431 (C8H6NO+), 138.05507 (C7H8NO2+), 180.06548 (C9H10NO3+), 246.07584 (C13H12NO4+), 248.12796 (C14H18NO3+), 264.08643 (C13H14NO5+), 282.09702 (C13H16NO6+), 392.17044 (C20H26NO7+), 410.18091 (C20H28NO8+)		
ascr	ubas#22	6.70	840.41309	100.03970 (C4H6NO2+), 103.05465 (C8H7+), 113.05997 (C6H9O2+), 120.08103 (C8H10N+), 129.06590 (C5H9N2O2+), 146.06020 (C9H8NO+), 156.08092 (C11H10N+), 157.06482 (C11H9O+),	838.29791	73.02834 (C3H5O2-), 85.02844 (C4H5O2-), 98.02380 (C4H4NO2-),102.05511 (C4H8NO2-), 113.05997 (C6H9O2-), 127.05063 (C5H7N2O2-),

				174.09148 (C11H12NO+), 184.07574 (C12H10NO+), 202.08629 (C12H12NO2+), 220.09645 (C12H14NO3+), 400.17545 (C22H26NO6+), 417.20221 (C22H29N2O6+), 460.20792 (C23H30N3O7+), 478.21887 (C23H32N3O8+), 592.28656 (C29H42N3O10+)		218.08241 (C12H12NO3-), 247.11870 (C11H19O6-), 261.13409 (C12H21O6-), 315.14471 (C15H23O7-), 332.17123 (C15H26NO7-), 375.17719 (C16H27N2O8-)
		6.85	289.15445	101.02367 (C4H5O3+), 117.07014 (C9H9+), 129.05466 (C6H9O3+), 143.07283 (C7H11O3+), 144.08076 (C10H10N+, major), 161.10722 (C10H13N2+), 243.11264 (C14H15N2O2+)		
ascr	pasy#1	6.88	495.27020	91.05466 (C7H7+), 103.05456 (C8H7+), 113.06003 (C6H9O2+), 120.08096 (C8H10N+), 146.06000 (C9H8NO+), 156.08075 (C11H10N+), 174.09137 (C11H12NO+), 184.07564 (C12H10NO+), 202.08624 (C12H12NO2+, major)		
ascr	ubas#23	6.91	865.45435	104.07088 (C4H10NO2+), 112.03951 (C5H6NO2+), 113.06001 (C6H9O2+), 115.07561 (C6H11O2+), 129.06590 (C5H9N2O2+), 130.04994 (C5H8NO3+), 147.07639 (C5H11N2O3+), 199.09647 (C10H15O4+), 242.10191 (C11H16NO5+), 259.12869 (C11H19N2O5+), 281.13821 (C15H21O5+), 341.17062 (C16H25N2O6+), 359.18127 (C16H27N2O7+)		
ascr	ubas#24	7.14	879.46985	104.07088 (C4H10NO2+), 112.03951 (C5H6NO2+), 113.06001 (C6H9O2+), 115.07561 (C6H11O2+), 129.06590 (C5H9N2O2+), 130.04994 (C5H8NO3+), 147.07639 (C5H11N2O3+), 199.09647 (C10H15O4+), 242.10191 (C11H16NO5+), 259.12869 (C11H19N2O5+), 295.15359 (C16H23O5+), 355.18622 (C17H27N2O6+), 373.19687 (C17H29N2O7+)		
ascr		7.14	782.45349	111.08079 (C7H11O+), 113.06005 (C6H9O2+), 129.09106 (C7H13O2+), 147.10152 (C7H5O3+), 183.13800 (C11H19O2+), 241.14357 (C13H21O4+), 259.15414 (C13H23O5+)	763.41299	73.02822 (C3H5O2-), 111.04437 (C6H7O2-), 127.07571 (C7H11O2-), 145.08650 (C7H13O3-), 275.14981 (C13H23O6-), 313.16589 (C16H25O6-), 505.26605 (C24H41O11-), 533.29700 (C26H45O11-)
		7.19	592.23932	120.04462 (C7H6NO+), 138.05502 (C7H8NO2+), 151.07547 (C9H11O2+), 154.06247 (C8H10O3+, rad), 169.08588 (C9H13O3+), 182.05743 (C9H10O4+, rad), 197.08096 (C10H13O4+), 228.06566 (C13H10NO3+), 293.13812 (C16H21O5+)		
		7.25	**309.13330**	see J2, ES+ table	307.11880	137.02379 (C7H5O3-), 165.01906 (C8H5O4-), 180.04272 (C9H8O4-, rad), 195.06618 (C10H11O4-)
ascr		7.33	673.29669	92.04996 (C6H6N+), 113.05995 (C6H9O2+), 120.04461 (C7H6NO+, major), 127.03910 (C6H7O3+), 129.09113 (C7H13O2+), 132.04446 (C8H6NO+), 138.05499 (C7H8NO2+), 172.07559 (C11H10NO+), 180.06546 (C9H10NO3+), 214.08633 (C13H12NO2+), 232.09679 (C13H14NO3+), 246.07600 (C13H12NO4+), 248.12796 (C14H18NO3+), 250.10699 (C13H16NO4+), 264.08679 (C13H14NO5+), 282.09689 (C13H16NO6+), 392.17035 (C20H26NO7+), 410.18082 (C20H28NO8+), 522.23236 (C26H36NO10+), 540.24353 (C26H38NO11+)	707.25889	73.02821 (C3H5O2-), 136.03966 (C7H6NO2-), 275.14999 (C13H23O6-)
		7.35	809.56207	see comments	439.24710, 449.27560	
		7.38	763.43427			
ascr	ubas#25	7.41	893.48523	83.08607 (C6H11+), 111.08073 (C7H11O+), 113.06001 (C6H9O2+), 129.06590		

				(C5H9N2O2+), 147.07646 (C5H11N2O3+), 199.09648 (C10H15O4+), 259.12878 (C11H19N2O5+), 309.16943 (C17H25O5+), 327.17978 (C17H27O6+), 387.21259 (C18H31N2O7+)		
		7.57	590.22327	81.03409 (C5H5O+), 97.02873 (C5H5O2+), 109.02865 (C6H5O2+), 120.04456 (C7H6NO+), 127.03915 (C6H7O3+), 138.05487 (C7H8NO2+), 146.02365 (C8H4NO2+), *195.10150 (C11H15O3+), *197.08087 (C10H15O4+), *199.07541 (C13H11O2+), *217.08582 (C13H13O3+), 228.06534 (C13H10NO3+), *231.10146 (C14H15O3+), *259.09622 (C15H15O4+), *263.12750 (C15H19O4+), *291.12247 (C16H19O5+), 309.13315 (C16H21O6+), 417.15475 (C22H25O8+), 435.16476 (C22H27O9+); (* fragments present in 309.13324)		
ascr	tasc#1	7.61	810.48486	see growth medium, ES- table		
		7.62	671.31781	105.07025 (C8H9+), 120.08096 (C8H10N+), 202.08669 (C12H12NO2+), 204.10181 (C12H14NO2+), 220.09677 (C12H14NO3+), 222.11235 (C12H16NO3+)	669.30331	
		8.03	545.47784	237.22112 (C16H29O+), 255.23164 (C16H31O2+)		
ascr		8.08	586.32245	151.07542 (C9H11O2+), 154.06252 (C8H10O3+, rad), 169.08588 (C9H13O3+), 182.05725 (C9H10O4+, rad), 197.08092 (C10H13O4+), 293.13824 (C16H21O5+)	567.28195	73.02826 (C3H5O2-), 127.07575 (C7H11O2-), 150.03191 (C8H6O3-, rad), 151.03966 (C8H7O3-), 165.05551 (C9H9O3-), 167.03479 (C8H7O4-), 168.04265 (C8H8O4-, rad), 275.14999 (C13H23O6-), 535.25525 (C28H39O10-)
		8.19	252.63503			
		8.51	704.29645	134.04654 (C5H4N5+), 165.02296 (C6H5N4S+), 182.04956 (C6H8N5S+), 194.04962 (C7H8N5S+), 250.11203 (C11H16N5S+)	702.28195	
ascr		8.57	584.30707	83.04971 (C5H7O+), 111.04443 (C6H7O2+), 113.05998 (C6H9O2+), 195.10184 (C11H15O3+), 197.08078 (C10H13O4+), 199.07579 (C13H11O2+), 217.08589 (C13H13O3+), 231.10155 (C14H15O3+), 259.09637 (C15H15O4+), 263.12762 (C15H19O4+), 277.10699 (C15H17O5+), 291.12259 (C16H19O5+), 309.13318 (C16H21O6+), 331.15421 (C19H23O5+), 389.15906 (C21H25O7+), 421.18558 (C22H29O8+)	565.26657	73.02825 (C3H5O2-), 127.07575 (C7H11O2-), 137.02380 (C7H5O3-), 165.01907 (C8H5O4-), 166.02692 (C8H6O4-, rad), 180.04277 (C9H8O4-, rad), 181.05055 (C9H9O4-), 195.06619 (C10H11O4-), 275.15005 (C13H23O6-)
ascr		8.91	844.46948	113.06007 (C6H9O2+), 129.09114 (C7H13O2+), 151.07542 (C9H11O2+), 154.06244 (C8H10O3+, rad), 169.08580 (C9H13O3+), 182.05734 (C9H10O4+, rad), 197.08087 (C10H13O4+), 293.13818 (C16H21O5+)	825.42898	73.02825 (C3H5O2-), 127.07559 (C7H11O2-), 139.03940 (C7H7O3-), 151.03940 (C8H7O3-), 167.03464 (C8H7O4-), 275.14981 (C13H23O6-), 533.29694 (dasc#1-), 793.40314 (C41H61O15-)
		8.93	702.28046	134.04654 (C5H4N5+), 165.02296 (C6H5N4S+), 182.04956 (C6H8N5S+), 194.04962 (C7H8N5S+), 250.11203 (C11H16N5S+)		
		9.64	770.46881	92.04996 (C6H6N+), 120.04459 (C7H6NO+), 138.05495 (C7H8NO2+), 248.12828 (C14H18NO3+), 264.08643 (C13H14NO5+), 282.09714 (C13H16NO6+), 392.17029 (C20H26NO7+), 410.18091 (C20H28NO8+)		
		10.14	474.32181	91.05473 (C7H7+), 119.04942 (C8H7O+), 151.07539 (C9H11O2+), 250.10728 (C13H16NO4+)		
		11.18	481.34277	144.08083 (C10H10N+), 156.08084 (C11H10N+), 243.11270 (C14H15N2O2+), 261.12341 (C14H17N2O3+), 382.31079		

				(C26H40NO+)		
		13.97	445.40402	see comments		
		14.34	459.41959	see comments		

Table S14. Differential metabolites from *P. pacificus* J2 medium, ES- mode, that are decreased or absent in RS2333 medium compared to RS2770 *Ppa-daf-22*. Entries that have a corresponding peak in the ES+ table are shaded grey.

class	*rt (min)*	*m/z (ES-)*	*MS/MS (ES-)*	*m/z (ES+)*	*MS/MS (ES+)*
	4.91	325.97858	see comments		
	4.91	243.12390	85.06474 (C6H9O-), 163.11259 (C11H15O-), 181.12338 (C11H17O2-), 199.13402 (C11H19O3-), 207.10269 (C12H15O3-), 225.11330 (C12H17O4-)		
	4.94	305.16074	59.01267 (C2H3O2-), 169.12321 (C10H17O2-), 171.10243 (C9H15O3-), 231.12366 (C11H19O5-)		
	5.22	215.16550			
	5.51	289.20248	59.01258 (C2H3O2-), 229.18105 (C13H25O3-)		
	5.71	301.20248	59.01258 (C2H3O2-), 241.18158 (C14H25O3-)		
	5.95	303.21808	59.01257 (C2H3O2-), 243.19644 (C14H27O3-)		
	5.96	421.24487	59.01259 (C2H3O2-, major), 71.01261 (C3H3O2-), 73.02825 (C3H5O2-), 83.01273 (C4H3O2-), 85.02836 (C4H5O2-), 101.02344 (C4H5O3-), 113.02362 (C5H5O3-)		
S	5.97	515.21716	59.01252 (C2H3O2-), 96.95906 (HSO4-), 353.16391 (C15H29SO7-)		
S	6.04	339.18475	96.95906 (HSO4-)		
	6.21	427.21051	59.01254 (C2H3O2-), 78.95783 (PO3-), 96.96854 (H2PO4-), 293.15286 (C13H26PO5-), 317.15231 (C15H26PO5-), 335.16373 (C15H28PO6-), 409.19943 (C18H34PO8-)		
S	6.48	353.16422	59.01255 (C2H3O2-), 96.95901 (HSO4-), 213.18600 (C13H25O2-), 273.20718 (C15H29O4-), 291.16360 (C14H27SO4-), 293.14294 (C13H25SO5-)		
	6.70	569.31000	78.95787 (PO3-), 96.96854 (H2PO4-)		
ascr	6.81	461.31259	59.01259 (C2H3O2-), 73.02829 (C3H5O2-)		
	6.84	315.21790	59.01256 (C2H3O2-), 85.06470 (C5H9O-), 115.07560 (C6H11O2-), 223.13402 (C13H19O3-), 241.14441 (C13H21O4-), 255.19650 (C15H27O3-), 297.20734 (C17H29O4-)		
S	6.90	293.14315	96.95601 (HSO4-)		
S	6.98	409.19031	59.01258 (C2H3O2-), 79.95618 (SO3-), 96.95906 (HSO4-), 329.23340 (C18H33O5-), 347.18964 (C17H31SO5-), 349.16904 (C16H29SO6-)		
	6.99	461.27621	59.01260 (C2H3O2-, major), 71.01255 (C3H3O2-), 73.02822 (C3H5O2-), 83.01260 (C4H3O2-), 85.02822 (C4H5O2-), 101.02342 (C4H5O3-)		
	7.34	259.19138	59.01256 (C2H3O2-), 199.17041 (C12H29O2-)	243.19543	
	7.41	447.26028	59.01256 (C2H3O2-, major), 71.01257 (C3H3O2-), 73.02827 (C3H5O2-), 83.01264 (C4H3O2-), 85.02834 (C4H5O2-), 101.02340 (C4H5O3-), 113.02355 (C5H5O3-)		
S	7.44	307.15847	96.95905 (HSO4-)		
	7.47	419.26532	59.01258 (C2H3O2-), 71.01259 (C3H3O2-), 73.02824 (C3H5O2-), 85.02828 (C4H5O2-), 101.02335 (C4H5O3-), 257.21225 (C15H29O3-)		
	7.62	327.21799	155.10748 (C9H15O2-), 171.10255 (C9H15O3-)		
	7.65	525.32037			
S	7.72	467.26859	59.01258 (C2H3O2-), 96.96905 (HSO4-), 327.29092 (C20H39O3-), 387.31192 (C22H43O5-), 405.26840 (C21H41SO5-), 407.24741 (C20H39SO6-)		
	7.87	273.20728	59.01258 (C2H3O2-, major), 213.18622 (C13H25O2-)		
S	8.01	341.11972	96.95901 (HSO4-), 305.14285 (C14H25SO5-)		
	8.06	271.19171	59.01258 (C2H3O2-)		
ascr	8.07	503.35956	59.01258 (C2H3O2-), 73.02826 (C3H5O2-), 83.04912 (C5H7O-), 111.04434 (C6H7O2-), 313.27481 (C19H37O3-)	505.37378	303.26807 (C21H35O+), 321.27896 (C21H37O2+), 339.28909 (C21H39O3+), 357.29959 (C21H41O4+)
S	8.16	481.28439	59.01257 (C2H3O2-), 96.96906 (HSO4-), 341.30609 (C21H41O3-), 401.32706 (C23H45O5-), 419.28345 (C22H43SO5-), 421.26300 (C21H41SO6-)		
ascr	8.49	517.37506	59.01258 (C2H3O2-), 73.02830 (C3H5O2-), 111.04440 (C6H7O2-), 327.29080 (C20H39O3-)	519.38934	317.28400 (C22H37O+), 335.29456 (C22H39O2+), 353.30545 (C22H41O3+)
ascr	8.95	531.39105	59.01259 (C2H3O2-), 73.02827 (C3H5O2-), 83.04907 (C5H7O-), 111.04420 (C6H7O2-), 341.30603 (C21H41O3-)		
ascr	8.95	445.31757	59.01262 (C2H3O2-), 73.02830 (C3H5O2-), 83.04909 (C5H7O-),		

			111.04427 (C6H7O2-), 255.23259 (C16H31O2-), 385.29572 (C22H41O5-)		
ascr	11.51	719.46021	59.01256 (C2H3O2-), 71.01259 (C3H3O2-), 73.02826 (C3H5O2-), 83.04903 (C5H7O-), 111.04431 (C6H7O2-), 511.40039 (C30H55O6-, major)		
	11.64	559.38599	335.33194 (C23H43O-), 379.32175 (C24H43O3-), 397.33215 (C24H45O4-)	578.42694	335.33081 (C23H43O+), 353.34134 (C23H45O2+), 381.33542 (C24H45O3+), 399.34692 (C24H47O4+)
ascr	12.57	747.49139	59.01260 (C2H3O2-), 71.01261 (C3H3O2-), 73.02826 (C3H5O2-), 83.04904 (C5H7O-), 111.04421 (C6H7O2-), 539.43158 (C32H59O6-, major)		
ascr	14.08	527.43207	71.01266 (C3H3O2-), 73.02832 (C3H5O2-), 83.04916 (C5H7O-), 111.04440 (C6H7O2-), 379.35822 (C25H47O2-), 397.36859 (C25H49O3-)		

Table S15. Differential metabolites from *P. pacificus* growth medium, ES- mode, that are decreased or absent in RS2333 medium compared to RS2770 *Ppa-daf-22*. Entries that have a corresponding peak in the ES+ table are shaded grey.

class	*smid-db*	*rt (min)*	*m/z (ES-)*	*MS/MS (ES-)*	*m/z (ES+)*	*MS/MS (ES+)*
		4.71	262.14514	91.05419 (C7H7-), 116.04967 (C8H6N-), 117.07011 (C9H9-), 118.06541 (C8H8N-), 143.04971 (C10H7O-), 162.05576 (C9H8NO2-), 201.12849 (C14H17O-), 245.11810 (C15H17O3-)	264.15961	91.05468 (C7H7+), 118.06532 (C8H8N+), 120.08092 (C8H10N+), 134.09641 (C9H12N+), 164.07048 (C9H10NO2+), 218.15387 (C14H20NO+)
S		4.83	355.17981	79.95612 (SO3-), 96.95904 (HSO4-)	357.19431	223.20566 (C15H27O+), 241.21605 (C15H29O2+), 259.22662 (C15H31O3+)
S		5.21	383.17496	59.01264 (C2H3O2-), 96.95904 (HSO4-), 243.19624 (C14H27O3-), 303.21768 (C16H31O5-), 321.17398 (C15H29SO5-), 323.15326 (C14H27SO6-)		
		5.25	537.19592	72.00785 (C2H2NO2-), 74.02358 (C2H4NO2-), 100.00299 (C3H2NO3-), 118.05016 (C4H8NO3-), 144.02969 (C6H2N5- or C5H6NO4-), *160.02620 (C6H5N5O-); (*) only in the 1st peak	539.21042	136.06183 (C5H6N5+), 162.04099 (C6H4N5O+), 281.09915 (C10H13N6O4+), 407.16733 (C17H23N6O6+)
	phesad#1,2	5.31	614.22247	1st peak: 72.00787 (C2H2NO2-), 74.02351 (C2H4NO2-), 100.00301 (C3H2NO3-), 118.05018 (C4H8NO3-), 144.02980 (C6H2N5- or C5H6NO4-), 160.02621 (C6H5N5O-); 2nd peak: 98.02369 (C4H4NO2-), 202.08746 (C12H12NO2-), 220.09796 (C12H14NO3-), 321.14569 (C16H21N2O5-)	616.23676	1st peak: 97.02882 (C5H5O2+), 136.06177 (C5H6N5+), 162.04095 (C6H4N5O+), 281.09909 (C10H13N6O4+), 318.13339 (C17H20NO5+); 2nd peak: 105.07020 (C8H9+), 138.05490 (C7H8NO2+), 156.06546 (C7H10NO3+), 162.04091 (C6H4N5O+), 166.04984 (C8H8NO3+), 184.06036 (C8H10NO4+), 204.10188 (C12H14NO2+), 263.08853 (C10H11N6O3+), 305.14938 (C16H21N2O4+), 323.15991 (C16H23N2O5+), 484.19366 (C22H26N7O6+)
S		5.34	369.19571	96.95902 (HSO4-)		
S		5.38	327.11230	96.95917 (HSO4-)		
		5.59	260.15054	74.02354 (C2H4NO2-), 84.04434 (C4H6NO-), 98.02377 (C4H4NO2-), 104.03442 (C3H6NO3-), 116.03461 (C4H6NO3-), 146.04556 (C5H8NO4-), 230.13992 (C11H20NO4-)	262.16504	
S		5.64	265.11172	96.95906 (HSO4-)		
		5.72	506.14349	78.95786 (PO3-), 96.96859 (H2PO4-), 148.96413 (C3H2PO5-), 223.00146 (C6H8PO7-), 241.01205 (C6H10PO8-), 369.09586 (C13H22PO10-), 378.05957 (C13H17NPO10-)		
S		5.74	326.12009	78.95785 (PO3-)	328.13459	75.02694 (C3H7S+), 230.15727 (C12H24NSO+)
S		5.77	353.16425	*59.01257 (C2H3O2-), 96.95894 (HSO4-), *213.18594 (C13H25O2-), 273.20721 (C15H29O4-), *291.16354 (C14H27SO4-), *293.14273 (C13H25SO5-); (*) only in 6.1-6.2 min peaks		
		5.86	231.16026	59.01258 (C2H3O2-), 171.13896 (C10H19O2-)		
S		5.88	501.23776	96.95898 (HSO4-), 321.17398 (C15H29SO5-), 339.18466 (C15H31SO6-)		
		5.89	339.14865	2nd peak: 96.05905 (HSO4-), 59.01258 (C2H3O2-), 259.19128 (C14H27O4-), 277.14771 (C13H25SO4-), 279.12701 (C12H23SO5-)		
		5.90	383.18427	78.95786 (PO3-), 96.96859 (H2PO4-)		
S		5.92	325.16934	96.95909 (HSO4-)		
		6.01	303.21802	59.01266 (C2H3O2-), 171.13881	305.23252	

				(C10H19O2-), 185.15445 (C11H12O2-), 243.19641 (C14H27O3-)		
		6.03	281.15240	78.95786 (PO3-)		
		6.09	455.18277	84.00805 (C3H2NO2-), 98.02377 (C4H4NO2-, main), 112.03960 (C5H6NO2-), 218.08224 (C12H12NO3-), 236.09285 (C12H14NO4-)	457.19751	101.02366 (C4H5O3+), 103.05452 (C8H7+), 120.08089 (C8H10N+), 146.05998 (C9H8NO+), 156.08073 (C11H10N+), 174.09123 (C11H12NO+), 184.07556 (C12H10NO+), 202.08612 (C12H12NO2+), 220.09668 (C12H14NO3+)
S		6.20	279.12717	96.95909 (HSO4-)		
S		6.20	353.20041	96.95905 (HSO4-)	372.24091	239.23676 (C16H31O+), 257.24728 (C16H33O2+), 275.25793 (C16H35O3+)
		6.28	272.15054	72.00786 (C2H2NO2-), 74.02351 (C2H4NO2-), 104.03435 (C3H6NO3-), 112.03949 (C5H6NO2-), 130.01372 (C4H4NO4-), 141.12796 (C9H17O-), 180.13937 (C11H18NO-), 242.13985 (C12H20NO4-)		
		6.34	716.18707	78.95783 (PO3-), 92.04948 (C6H6N-), 96.96855 (H2PO4-), 98.02369 (C4H4NO2-), 136.03979 (C7H6NO2-), 148.96419 (C3H2PO5-), 218.08224 (C12H12NO3-), 223.00133 (C6H8PO7-), 236.09312 (C12H14NO4-), 442.09055 (C18H21NPO10-), 579.13934 (C25H28N2PO12-)	718.20157	103.05465 (C8H7+), 120.08099 (C8H10N+), 127.03903 (C6H7O3+), 143.03401 (C6H7O4+), 146.05991 (C9H8NO+), 156.08102 (C11H10N+), 174.09132 (C11H12NO+), 184.07582 (C12H10NO+), 202.08632 (C12H12NO2+), 220.09680 (C12H14NO3+), 262.10745 (C14H16NO4+), 328.11807 (C18H18NO5+), 346.12848 (C18H20NO6+)
S		6.37	339.18448	96.95905 (HSO4-)		
		6.38	433.19989	78.95783 (PO3-), 96.96855 (H2PO4-)	435.21439	
		6.39	679.19122	78.95785 (PO3-)	681.20572	1st peak: 105.07027 (C8H9+), 120.08101 (C8H10N+), 146.06013 (C9H8NO+), 183.07625 (C8H11N2O3+), 204.10197 (C12H14NO2+); 2nd peak: 120.08097 (C8H10N+), 202.08623 (C12H12NO2+), 328.11795 (C18H18NO5+), 346.12845 (C18H20NO6+)
		6.39	490.14890		492.16340	
		6.51	681.20752	78.95779 (PO3-), 136.03993 (C7H6NO2-), 148.96431 (C3H2PO5-), 223.00121 (C6H8PO7-), 442.09048 (C18H21NPO10-), 544.15948 (C23H31NPO12-)	683.22202	103.05449 (C8H7+), 109.02869 (C6H5O2+), 120.08091 (C8H10N+), 127.03893 (C6H7O3+), 156.08086 (C11H10N+), 174.09131 (C11H12NO+), 184.07600 (C12H10NO+), 202.08623 (C12H12NO2+), 220.09679 (C12H14NO3+), 262.10663 (C14H16NO4+), 328.11755 (C18H18NO5+), 346.12836 (C18H20NO6+), 430.18597 (C23H28NO7+), 528.16199 (C23H31NPO11+)
S		6.68	293.14319	96.95909 (HSO4-)		
S		6.71	367.17947	59.01259 (C2H3O2-), 96.95898 (HSO4-), 287.22290 (C16H31O4-), 305.17926 (C15H29SO4-), 307.15875 (C14H27SO5-), 309.17374 (C14H29SO5-)		
S		6.71	409.19016	59.01256 (C2H3O2-), 79.95615 (SO3-), 96.95903 (HSO4-), 155.10718 (C9H15O2-), 207.06949 (C8H15SO4-), 215.12903 (C11H19O4-), 235.06493 (C9H15SO5-), 311.22299 (C18H31O4-), 329.23346 (C18H33O5-), 347.18970 (C17H31SO5-), 349.16901 (C16H29SO6-)		
		6.76	363.19418	78.95782 (PO3-), 96.96853 (H2PO4-)	365.20868	267.23169 (C17H31O2+)

		7.16	387.19424	78.95783 (PO3-), 96.96855 (H2PO4-)	389.20874	
		7.36	403.22531	78.95786 (PO3-), 96.96851 (H2PO4-), 385.21561 (C20H34PO5-)		
		7.62	333.18332	78.95783 (PO3-), 96.96855 (H2PO4-)	335.19782	
S		7.68	363.18478	79.95628 (SO3-), 96.95913 (HSO4-), 207.06972 (C8H15SO4-), 249.08029 (C10H17SO5-)		
		7.95	693.24384	78.95785 (PO3-), 92.04948 (C6H6N-), 96.96854 (H2PO4-), 98.02382 (C4H4NO2-), 136.03990 (C7H6NO2-), 148.96414 (C3H2PO5-), 202.08759 (C12H12NO2-), 220.09807 (C12H14NO3-), 223.00159 (C6H8PO7-), 426.09634 (C18H21NPO9-), 444.10687 (C18H23NPO10-), 556.19562 (C25H35NPO11-), 581.15302 (C25H30N2PO12-)		
ascr		8.19	539.29938	59.01258 (C2H3O2-), 78.95785 (PO3-), 96.96854 (H2PO4-), 209.02216 (C6H10PO6-)		
		8.27	349.21518	78.95785 (PO3-), 96.96854 (H2PO4-)	351.22968	
S		8.37	675.41864	96.95901 (HSO4-)		
		8.47	287.22305	59.01255 (C2H3O2-), 227.20172 (C14H27O2-)	289.23755	
S		8.55	347.19022	96.95904 (HSO4-)		
		8.72	635.40228	59.01258 (C2H3O2-), 71.01259 (C3H3O2-), 73.02824 (C3H5O2-), 85.02831 (C4H5O2-), 101.02331 (C4H5O3-), 113.02348 (C5H5O3-), 247.17030 (C16H32O2-), 299.22290 (C17H31O4-), 335.22302 (C20H31O4-)	654.44278	249.25749 (C18H33+), 267.26807 (C18H35O+), 273.25751 (C20H33+), 291.26794 (C20H35O+), 309.27838 (C20H37O2+), 327.28918 (C20H39O3+), 345.29990 (C20H41O4+)
ascr		8.73	553.31543	59.01258 (C2H3O2-), 78.95785 (PO3-), 96.96854 (H2PO4-), 209.02216 (C6H10PO6-)	555.32993	211.03668 (C6H12PO6+), 267.26807 (C18H35O+), 291.26831 (C20H35O+), 309.27869 (C20H37O2+), 327.28915 (C20H39O3+)
S		8.89	363.22137	96.95904 (HSO4-)		
		8.89	301.23862	59.01262 (C2H3O2-), 241.21727 (C15H29O2-)		
		8.91	513.22607	83.01268 (C4H3O2-), 315.19659 (C20H27O3-)	479.26387	
S		8.91	351.22128	96.95908 (HSO4-)		
		8.93	385.29611	see comments	387.31061	
		8.93	359.28055			
ascr		8.94	531.39044	59.01259 (C2H3O2-), 73.02827 (C3H5O2-), 83.04910 (C5H7O-), 111.04434 (C6H7O2-), 341.30606 (C21H41O3-), 471.36911 (C27H51O6-), 513.37927 (C29H53O7-)	533.40494	
		8.94	337.23871	59.01259 (C2H3O2-)		
S		8.94	377.20062	96.95910 (HSO4-), 183.13878 (C11H19O2-), 297.24332 (C18H33O3-)		
ascr		8.94	445.31720	59.01258 (C2H3O2-), 73.02825 (C3H5O2-), 83.04906 (C5H7O-), 111.04426 (C6H7O2-), 255.23299 (C16H31O2-), 385.29578 (C22H41O5-), 427.30646 (C24H43O6-)		
		8.97	624.25842	179.14406 (C12H19O-), 223.13402 (C13H19O3-)	590.29622	105.07022 (C8H9+), 204.10191 (C12H14NO2+), 222.11235 (C12H16NO3+), 225.14845 (C13H21O3+), 330.13330 (C18H20NO5+), 348.14413 (C18H22NO6+), 366.15485 (C18H24NO7+)
		9.03	313.23862	1st peak: 59.01259 (C2H3O2-, major), 99.08060 (C6H11O-), 129.09145 (C7H13O2-), 183.13899 (C11H19O2-); 2nd peak: 59.01259 (C2H3O2-, major), 139.11230 (C9H15O-); 3rd peak: 59.01259 (C2H3O2-, major), 99.08055	315.25312	

				(C6H11O-), 253.21727 (C16H29O2-)		
		9.05	557.38116	70.02860 (C3H4NO-), 73.02827 (C3H5O2-), 96.00805 (C4H2NO2-), 113.03478 (C4H5N2O2-), 114.01889 (C4H4NO3-), 131.04562 (C4H7N2O3-), 294.28058 (19H36NO-), 299.22314 (C17H31O4-), 312.29120 (C19H38NO2-), 539.36987 (C29H51N2O7-)		
		9.06	473.23950	221.19110 (C15H25O-), 223.17035 (C14H23O2-), 265.18085 (C16H25O3-)		
		9.09	374.29156	59.01259 (C2H3O2-), 328.28632 (C19H38NO3-)		
		9.16	649.41772			
ascr		9.29	567.33087	78.95786 (PO3-), 96.96858 (H2PO4-), 209.02220 (C6H10PO6-)	569.34537	211.03659 (C6H12PO6+), 263.27322 (C19H35+), 281.28378 (C19H37O+), 287.27365 (C21H35+), 305.28397 (C21H37O+), 323.29428 (C21H39O2+), 341.30502 (C21H41O3+)
		9.31	257.21246			
		9.36	267.19678	99.08057 (C6H11O-), 205.19635 (C15H25-)	269.21128	
		9.39	545.40631	59.01259 (C2H3O2-), 73.02828 (C3H5O2-), 341.30676 (C21H41O3-)	547.42081	345.31500 (C24H41O+), 363.32535 (C24H43O2+), 381.33627 (C24H45O3+)
		9.44	399.31171	59.01258 (C2H3O2-)	401.32621	
		9.50	499.25537	59.01262 (C2H3O2-), 71.01260 (C3H3O2-), 89.02328 (C3H5O3-), 101.02344 (C4H5O3-), 113.02354 (C5H5O3-), 247.20692 (C17H27O-), 291.19672 (C18H27O3-)		
ascr		9.51	459.33325	59.01258 (C2H3O2-), 73.02825 (C3H5O2-), 83.04906 (C5H7O-), 111.04426 (C6H7O2-), 269.24881 (C17H33O2-)		
ascr		9.54	661.41791	59.01260 (C2H3O2-), 73.02826 (C3H5O2-), 83.04905 (C5H7O-), 111.04420 (C6H7O2-), 309.28009 (C20H37O2-), 325.31119 (C21H41O2-), 455.37424 (C27H51O5-), 499.36420 (C28H51O7-)	680.45841	
		9.56	571.39697	58.02855 (C2H4NO-), 70.02858 (C3H4NO-), 73.02825 (C3H5O2-), 96.00804 (C4H2NO2-), 113.03481 (C4H5N2O2-), 114.01881 (C4H4NO3-), 131.04555 (C4H7N2O3-), 292.26456 (C19H34NO-), 306.28052 (C20H36NO-), 308.29666 (C20H38NO-), 326.30661 (C20H40NO2-), 456.36880 (C26H50NO5-), 553.38666 (C30H53N2O7-)		
		9.57	605.39172		624.43222	
S		9.57	422.25070		388.28850	75.02692 (C3H7S+), 261.22113 (C18H29O+), 304.26331 (C20H34NO+), 322.27380 (C20H36NO2+), 352.26666 (C21H38NSO+), 370.27725 (C21H40NSO2+)
		9.61	339.25436	59.01257 (C2H3O2-, main), 113.09641 (C7H13O-), 165.12837 (C11H17O-), 321.24377 (C20H33O4-)		
ascr		9.67	663.43311	59.01256 (C2H3O2-), 71.01259 (C3H3O2-), 85.02834 (C4H5O2-), 101.02341 (C4H5O3-), 113.02361 (C5H5O3-), 645.42188 (C34H61O11-)	682.47375	277.28876 (C20H37+), 295.29932 (C20H39O+), 301.28885 (C22H37+), 319.29941 (C22H39O+), 337.30997 (C22H41O2+), 355.32043 (C22H43O3+), 373.33087 (C22H45O4+)
		9.68	830.52301			
		9.68	780.54041	267.23297 (C17H31O2-), 464.27826 (C22H43NPO7-)		
		9.88	315.25430	59.01257 (C2H3O2-), 255.23308 (C16H31O2-)		

ascr		9.99	725.42590	73.02826 (C3H5O2-), 83.04905 (C5H7O-), 111.04420 (C6H7O2-), 353.34268 (C23H45O2-), 483.40588 (C29H55O5-), 527.39545 (C30H55O7-)	708.48975	9.89 min: 289.28891 (C21H37+), 317.32007 (C23H41+), 345.31512 (C24H41O+), 363.32574 (C24H43O2+); 10.44 min: 233.18999 (C16H25O+), 277.21597 (C18H29O2+), 303.30457 (C22H39+), 321.24231 (C20H33O3+), 345.31430 (C24H41O+), 363.32556 (C24H43O2+), 381.33640 (C24H45O3+); 10.62 and 10.68 min: 289.28879 (C21H37+), 307.29932 (C21H39O+), 345.31430 (C24H41O+), 363.32556 (C24H43O2+), 381.33640 (C24H45O3+); 10.82 and 10.88 min: 289.28879 (C21H37+), 307.29932 (C21H39O+), 363.32556 (C24H43O2+), 381.33640 (C24H45O3+), 399.34662 (C24H47O4+)
		10.00	341.26993	59.01257 (C2H3O2-)		
		10.07	585.41260	1st peak: 73.02831 (C3H5O2-), 109.03986 (C5H5N2O-), 127.05058 (C5H7N2O2-), 145.06140 (C5H9N2O3-), 393.34906 (C24H45N2O2-); 2nd peak: 70.02860 (C3H4NO-), 73.02827 (C3H5O2-), 96.00805 (C4H2NO2-), 114.01885 (C4H4NO3-), 131.04556 (C4H7N2O3-), 306.27991 (C20H36NO-), 320.29584 (C21H38NO-), 322.31171 (C21H40NO-), 340.32217 (C21H42NO2-), 470.38571 (C27H52NO5-), 567.40100 (C31H55N2O7-)	587.42710	1st peak: 129.06592 (C5H9N2O2+), 130.04988 (C5H8NO3+), 147.07634 (C5H11N2O3+), 439.35269 (C25H47N2O4+)
ascr		10.09	581.34662	78.95783 (PO3-), 96.96855 (H2PO4-), 209.02213 (C6H10PO6-)	583.36112	211.03670 (C6H12PO6+), 277.28891 (C20H37+), 295.29950 (C20H39O+), 301.28879 (C22H37+), 319.29980 (C22H39O+), 337.31030 (C22H41O2+), 355.32037 (C22H43O3+)
ascr		10.17	677.44861	59.01259 (C2H3O2-), 71.01259 (C3H3O2-), 73.02824 (C3H5O2-), 85.02833 (C4H5O2-), 101.02332 (C4H5O3-), 113.02345 (C5H5O3-)	696.48914	291.30435 (C21H39+), 309.31503 (C21H41O+), 315.30453 (C23H39+), 333.31494 (C23H41O+), 351.32556 (C23H43O2+), 369.33630 (C23H45O3+), 387.34702 (C23H47O4+)
		10.18	473.34872	59.01260 (C2H3O2-), 73.02826 (C3H5O2-), 83.04905 (C5H7O-), 111.04420 (C6H7O2-), 283.26422 (C18H35O2-), 413.32745 (C24H45O5-), 455.33817 (C26H47O6-)	492.38922	249.25754 (C18H33+), 267.26807 (C18H35O+), 273.25751 (C20H33+), 291.26804 (C20H35O+), 309.27869 (C20H37O2+), 327.28922 (C20H39O3+)
		10.24	491.24237	249.22238 (C17H29O-), 251.20169 (C16H27O2-), 293.21246 (C18H29O3-)	457.28017	295.22672 (C18H31O3+)
		10.34	503.28690	83.01271 (C4H3O2-), 295.22775 (C18H31O3-)	459.29590	
ascr		10.58	487.36447	59.01256 (C2H3O2-), 73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 297.27982 (C19H37O2-), 427.34311 (C25H47O5-), 469.35345 (C27H49O6-)	506.40527	263.27307 (C19H35+), 291.28366 (C19H37O+), 287.27310 (C21H35+), 305.28354 (C21H37O+), 323.29419 (C21H39O2+), 341.30478 (C21H41O3+)
ascr		10.58	737.47083	73.02826 (C3H5O2-, main), 325.31134 (C21H41O2-), 455.37424 (C27H51O5-), 529.41095 (C30H57O7-)	710.50494	291.30426 (C21H39+), 309.31506 (C21H41O+), 329.32022 (C24H41+), 347.33072 (C24H43O+), 365.34149 (C24H45O2+), 383.35181 (C24H47O3+), 401.36224 (C24H49O4+)

ascr		10.62	507.30951	78.95783 (PO3-), 96.96855 (H2PO4-)	509.32401	211.03656 (C6H12PO6+), 263.27313 (C19H35+), 281.28372 (C19H37O+)
		10.63	343.28574	59.01257 (C2H3O2-), 283.26434 (C18H35O2-)		
ascr		10.66	639.38892		622.45288	277.28876 (C20H37+), 295.29929 (C20H39O+); 2nd peak also has 313.30991 (C20H41O2+)
ascr		10.69	537.32037	78.95783 (PO3-), 96.96857 (H2PO4-), 209.02222 (C6H10PO6-)	539.33487	113.06002 (C6H9O2+), 211.03665 (C6H12PO6+), 275.27356 (C20H35+), 293.28381 (C20H37O+), 311.29385 (C20H39O2+)
ascr		10.71	681.39966	483.36929 (C28H51O6-)	664.46346	319.29941 (C22H39O+), 337.30988 (C22H41O2+)
ascr		10.79	529.41119	1st peak: 73.02827 (C3H5O2-), 399.34814 (C24H47O4-); 2nd and 3rd peaks: 73.02827 (C3H5O2-, main); 4th peak: 59.01257 (C2H3O2-, main), 73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 339.32684 (C22H43O2-), 469.38995 (C28H53O5-), 511.40085 (C30H55O6-)	531.42569	2nd and 3rd peaks: 309.31497 (C21H41O+), 329.31985 (C24H41+), 347.33066 (C24H43O+), 365.34146 (C24H45O2+); 4th peak: 305.32007 (C22H41+), 323.33060 (C22H43O+), 329.31967 (C24H41+), 347.33105 (C24H43O+), 365.34155 (C24H45O2+)
ascr		10.92	693.44373	355.32211 (C22H43O3-), 485.38556 (C28H53O6-)	666.47873	321.31509 (C22H41O+), 339.32581 (C22H43O2+)
		11.06	369.30115	59.01257 (C2H3O2-), 309.28046 (C20H37O2-)		
ascr		11.07	703.46478	73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 367.35794 (C24H47O2-), 497.42142 (C30H57O5-), 541.41138 (C31H57O7-)		
		11.12	613.44366	1st peak: 73.02827 (C3H5O2-), 109.03986 (C5H5N2O-), 127.05059 (C5H7N2O2-), 145.06123 (C5H9N2O3-), 421.38019 (C26H49N2O2-); 2nd peak: 70.02860 (C3H4NO-), 73.02836 (C3H5O2-), 96.00813 (C4H2NO2-), 114.01888 (C4H4NO3-), 131.04559 (C4H7N2O3-), 334.31137 (C22H40NO-), 348.32715 (C23H42NO-), 350.34302 (C23H44NO-), 368.35339 (C23H46NO2-), 595.43219 (C33H59N2O7-)	615.45816	
ascr		11.13	501.38013	59.01259 (C2H3O2-, main), 71.01263 (C3H3O2-), 73.02828 (C3H5O2-), 83.04910 (C5H7O-), 111.04433 (C6H7O2-), 311.29605 (C20H39O2-), 441.35944 (C26H49O5-), 483.36813 (C28H51O6-)	503.39465	277.28864 (C20H37+), 295.29922 (C20H39O+), 301.28864 (C22H37+), 319.29929 (C22H39O+), 337.30991 (C22H41O2+), 355.32031 (C22H43O3+)
		11.19	397.30746	73.03945 (C2H5N2O-), 130.08653 (C6H12NO2-), 143.11835 (C7H15N2O-), 187.10893 (C8H15N2O3-), 226.21767 (C14H28NO-), 266.21240 (C16H28NO2-), 353.31763 (C21H41N2O2-)		
		11.20	565.35181	367.32227 (C23H43O3-)	548.41561	
		11.37	641.47571	73.02831 (C3H5O2-), 109.03984 (C5H5N2O-), 127.05057 (C5H7N2O2-), 128.03456 (C5H6NO3-), 145.06151 (C5H9N2O3-), 449.41101 (C28H53N2O2-)	643.49011	129.06598 (C5H9N2O2+), 130.04996 (C5H8NO3+), 147.07648 (C5H11N2O3+), 495.41556 (C29H55N2O4+), 513.42761 (C29H57N2O5+)
		11.50	787.44684			
ascr		11.51	709.43085	73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 511.40039 (C30H55O6-)	692.49469	291.30438 (C21H39+), 319.33585 (C23H43+), 329.32010 (C24H41+), 347.33069 (C24H43O+), 365.34128 (C24H45O2+)
		11.53	383.31683	59.01259 (C2H3O2-)		
		11.57	371.31689	59.01259 (C2H3O2-)		
ascr		11.61	457.35400	73.02823 (C3H5O2-), 327.29065 (C20H39O3-)		
ascr		11.66	765.50146	73.02823 (C3H5O2-, main), 557.44226	738.53646	319.33600 (C23H43+), 337.34692

				(C32H61O7-)		(C23H45O+), 357.35135 (C26H45+), 375.36212 (C26H47O+), 393.37250 (C26H49O2+), 411.38321 (C26H51O3+), 429.39420 (C26H53O4+)
ascr		11.67	515.39551	59.01263 (C2H3O2-, main), 73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 325.31146 (C21H41O2-)	534.43719	291.30435 (C21H39+), 309.31488 (C21H41O+), 315.30414 (C23H39+), 333.31497 (C23H41O+), 351.32535 (C23H43O2+), 369.33606 (C23H45O3+)
		11.68	579.36743	381.33746 (C24H45O3-)	567.38733	185.04196 (C6H10O5Na+), 405.33371 (C24H46O3Na+)
ascr		11.69	557.44257	11.67 - 11.80 min: 73.02827 (C3H5O2-), 409.36914 (C26H49O3-), 427.37970 (C26H51O4-); 12.94 and 13.05 min: 73.02826 (C3H5O2-), 111.04430 (C6H7O2-), 353.34299 (C23H45O2-); 13.19 min: 59.01257 (C2H3O2-, main), 73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 367.35941 (C24H47O2-); 13.39 min: 73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 381.37427 (C25H49O2-)	581.43884	
ascr		11.77	711.44617	73.02790 (C3H5O2-), 383.35321 (C24H47O3-), 513.41626 (C30H57O6-)	694.51080	331.33572 (C24H43+), 349.34637 (C24H45O+), 367.35690 (C24H47O2+)
		11.91	397.33255	59.01258 (C2H3O2-)		
ascr		12.12	471.36945	73.02827 (C3H5O2-), 341.30612 (C21H41O3-)		
ascr		12.55	737.46240	73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 539.43182 (C32H59O6-)	720.52612	319.33588 (C23H43+), 347.36722 (C25H47+), 357.35162 (C26H45+), 375.36215 (C26H47O+), 393.37265 (C26H49O2+)
ascr		12.61	485.38525	73.02828 (C3H5O2-), 337.31149 (C22H41O2-), 355.32196 (C22H43O3-)		
ascr		12.69	643.35297			
ascr		12.70	497.38541	73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-)		
ascr		12.80	739.47815	73.2825 (C3H5O2-), 411.38498 (C26H51O3-), 541.44745 (C32H61O6-)	722.54144	359.36719 (C26H47+), 377.37781 (C26H49O+), 395.38840 (C26H51O2+)
ascr		13.09	499.40103	73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 351.32697 (C23H43O2-), 369.33743 (C23H45O3-)	371.35159	317.32004 (C23H41+), 335.33066 (C23H43O+)
ascr		13.10	511.40070	see comments		
ascr		13.19	593.38312	see comments		
ascr		13.47	513.41626	see comments		
ascr		13.69	571.45831	59.01258 (C2H3O2-, main), 73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-), 381.37387 (C25H49O2-), 511.43588 (C31H59O5-), 553.44769 (C33H61O6-)	595.45496	
ascr		14.08	527.43188	73.02827 (C3H5O2-), 379.35855 (C25H47O2-), 397.36871 (C25H49O3-)		
ascr		14.25	585.47430	59.01258 (C2H3O2-)		
ascr		14.49	539.43207	73.02823 (C3H5O2-), 83.04904 (C5H7O-), 111.04424 (C6H7O2-); 2nd (bigger) peak also has 409.36911 (C26H49O3-)		
ascr		14.53	541.44763	73.02826 (C3H5O2-), 393.37390 (C26H49O2-), 411.38440 (C26H51O3-)		

Table S16. Differential metabolites from *P. pacificus* J2 medium, ES+ mode, which are decreased or absent in RS2333 medium compared to RS2770 *Ppa-daf-22*. Entries that have a corresponding peak in the ES- table are shaded grey.

class	*rt (min)*	*m/z (ES+)*	*MS/MS (ES+)*	*m/z (ES-)*
	1.81	227.21188	84.08137 (C5H10N+), 127.12311 (C7H15N2+)	
	3.75	228.19603	70.06582 (C4H8N+)	
	4.69	330.22775	60.08158 (C3H10N+), 85.02898 (C4H5O2+), 123.11700 (C9H15+), 253.14320 (C14H21O4+)	
	4.90	209.11752	91.05471 (C7H7+), 93.07034 (C7H9+), 105.07021 (C8H9+), 107.04953 (C7H7O+), 111.04430 (C6H7O2+), 113.06002 (C6H9O2+), 115.03898 (C5H7O3+), 117.07011 (C9H9+), 121.06493 (C8H9O+), 125.05984 (C7H9O2+), 131.08556 (C10H11+), 145.10117 (C11H13+), 149.09616 (C10H13O+), 163.11168 (C11H15O+), 173.09612 (C12H13O+), 191.10660 (C12H15O2+)	
	5.05	268.22708	59.04993 (C3H7O+), 70.06580 (C4H8N+), 117.09119 (C6H13O2+)	
	5.05	237.14612		
	5.38	553.22559	136.06177 (C5H6N5+), 162.04094 (C6H4N5O+), 281.09906 (C10H13N6O4+)	
	5.70	283.15173		
	5.74	285.16727		
	5.76	320.27957	60.04520 (C2H6NO+), 90.05543 (C3H8NO2+), 266.24768 (C17H32NO+), 284.25864 (C17H34NO2+), 302.26859 (C17H36NO3+)	
	5.80	212.20108	70.06580 (C4H8N+)	
S	6.38	434.15234	56.96559 (CaOH+), 277.14761 (C15H25O2Ca+), 295.15775 (C15H27O3Ca+), 393.12552 (C15H29SO7Ca+)	
	6.47	304.28458	60.04521 (C2H6NO+), 250.25275 (C17H32N+), 268.26328 (C17H34NO+), 286.27380 (C17H36NO2+)	
	6.56	239.20064	203.17934 (C15H23+), 221.18953 (C15H25O+)	
	6.74	394.28000	197.19002 (C13H25O+)	
S	6.85	364.25153	86.06055 (C4H8NO+), 90.03766 (C3H8NS+), 98.06041 (C5H8NO+), 108.04806 (C3H10NSO+), 264.23196 (C17H30NO+), 282.24246 (C17H32NO2+), 300.25320 (C17H34NO3+), 328.23022 (C18H34NSO2+), 346.24072 (C18H36NSO3+)	
	7.10	413.22995		
	7.20	412.30609	85.02898 (C4H5O2+)	
	7.20	347.27908		
	7.26	243.19543		259.19138
S	7.34	262.18344	90.03763 (C3H8NS+), 108.04813 (C3H10NSO+), 192.13832 (C12H18NO+), 198.18526 (C12H24NO+, major), 244.17302 (C13H26NSO+)	
	7.41	420.29535		
	7.60	491.35800	265.25238 (C18H33O+), 289.25296 (C20H3O+), 307.26321 (C20H35O2+), 325.27411 (C20H37O3+), 411.30875 (C24H43O5+)	
	7.78	502.37393	85.02898 (C4H5O2+)	
	7.78	257.21091		
	7.79	524.33490	60.08155 (C3H10N+), 86.09694 (C5H12N+), 104.10734 (C5H14NO+), 124.99993 (C2H6PO4+), 184.07323 (C5H15NPO4+), 506.32437 (C25H49NPO7+)	
	7.85	434.31131		
	8.03	287.25806	233.22620 (C17H29+), 251.23708 (C17H31O+), 269.24734 (C17H33O2+)	
	8.04	407.25571	291.26801 (C20H35O+), 309.27878 (C20H37O2+)	
	8.05	574.43170	85.02895 (C4H5O2+), 444.36792 (C25H50NO5+)	
	8.06	505.37378	see J2, ES- table	
	8.07	253.21605	217.19522 (C16H25+), 235.20601 (C16H25O+)	
	8.39	453.31863		
	8.51	530.40533	60.08159 (C3H10N+), 85.02897 (C4H5O2+, major)	
	8.52	519.38934	see J2, ES- table	
	8.52	588.44733	60.08158 (C3H10N+), 85.02898 (C4H5O2+), 113.06007 (C6H9O2+), *144.10193 (C7H14NO2+), 381.30011 (C23H41O4+), 458.38397 (C26H52NO5+); (*) 1st peak only	
	8.86	544.42090		
	8.86	702.47913	85.02898 (C4H5O2+), 540.42676 (C31H58NO6+)	
	8.89	445.35223		
	8.94	602.46307	60.08160 (C3H10N+), 85.02898 (C4H5O2+), 113.06005 (C6H9O2+), 144.10191 (C7H14NO2+), 395.31558 (C24H43O4+), 472.39993 (C27H54NO5+)	
	9.22	558.43604	85.02898 (C4H5O2+)	
	9.30	616.47815	60.08157 (C3H10N+), 85.02895 (C4H5O2+), 113.05997 (C6H9O2+), 144.10197 (C7H14NO2+), 409.33170 (C25H45O4+), 486.41519 (C28H56NO5+)	
	9.49	309.23987		
	9.52	630.49396	60.08157 (C3H10N+), 85.02895 (C4H5O2+), 113.06001 (C6H9O2+), 144.10190 (C7H14NO2+),423.34619 (C26H47O4+), 500.43112 (C29H58NO5+)	
	9.62	295.26306	277.25256 (C19H33O+)	

S	10.00	580.38794	60.08154 (C3H10N+), 85.02892 (C4H5O2+), 500.43079 (C29H58NO5+)	
	11.63	578.42694	see J2, ES- table	
ascr	11.79	692.49506	85.02901 (C4H5O2+), 113.06002 (C6H9O2+), 131.07031 (C6H11O3+), 347.33087 (C24H43O+), 365.34137 (C24H45O2+)	
ascr	12.00	694.51050	85.02901 (C4H5O2+), 113.06005 (C6H9O2+), 131.07040 (C6H11O3+), 349.34653 (C24H45O+), 367.35718 (C24H47O2+)	
	12.20	569.40314	185.04205 (C6H10O5Na+), 407.34955 (C24H48O3Na)	
	12.24	385.36783	349.34641 (C24H45O+)	
ascr	12.56	720.52612	85.02896 (C4H5O2+), 113.06000 (C6H9O2+), 131.07036 (C6H11O3+), 145.04965 (C6H9O4+), 375.36206 (C26H47O+), 393.37256 (C26H49O2+)	
	12.64	516.42639	333.31506 (C23H41O+), 351.32578 (C23H43O2+)	
	12.70	415.37823	361.34683 (C25H45O+), 379.35663 (C25H47O2+)	
	12.71	567.42346		
	12.76	553.40765		
	12.79	795.41119		
ascr	12.81	722.54187	85.02896 (C4H5O2+), 113.05998 (C6H9O2+), 131.07031 (C6H11O3+), 145.04958 (C6H9O4+), 377.37762 (C26H49O+), 395.38821 (C26H51O2+), 457.40408 (C31H53O2+), 485.39835 (C32H53O3+), 503.40921 (C32H55O4+), 521.41998 (C32H57O5+), 539.43091 (C32H59O6+)	
	12.97	611.44952		
	13.07	353.34119		
	13.07	535.39716		
	13.14	595.41821	433.36670 (C26H50O3Na+)	
	13.20	581.43903		
	13.22	565.40771		
	13.69	595.45483	465.39206 (C27H54O4Na+)	
	13.77	637.46533		
	14.04	593.43927		
	14.07	595.45477		
	14.17	521.41797		
	14.40	577.44415		

Table S17. Differential metabolites from *P. pacificus* growth medium, ES+ mode, that are decreased or absent in RS2333 medium compared to RS2770 *Ppa-daf-22*. Entries that have a corresponding peak in the ES- table are shaded grey.

class	*rt (min)*	*m/z (ES+)*	*MS/MS (ES+)*
	1.41	215.21175	84.08131 (C5H10N+), 86.09692 (C5H12N+), 98.09678 (C6H12N+), 115.12318 (C6H15N2+), 198.18513 (C12H24NO+)
	3.26	322.14948	94.06552 (C6H8N+), 96.08115 (C6H10N+), 100.03961 (C4H6NO2+), 102.05526 (C4H8NO2+), 103.03926 (C4H7O3+), 112.07576 (CC6H10NO+), 114.09156 (C6H12NO+), 117.05482 (C5H9O3+), 118.08642 (C5H12NO2+), 124.07586 (C7H10NO+), 131.03392 (C5H7O4+), 142.08620 (C7H12NO2+), 145.04958 (C6H9O4+), 156.10188 (C8H14NO2+), 174.11234 (C8H16NO3+), 202.10733 (C9H16NO4+), 216.12297 (C10H18NO4+), 262.12827 (C11H20NO6+), 276.14389 (C12H22NO6+)
	3.76	243.20668	84.08131 (C5H10N+), 114.09158 (C6H12NO+), 143.11786 (C7H15N2O+)
	3.79	216.15955	70.06581 (C4H8N+), *87.04457 (C4H7O2+), 98.06045 (C5H8NO+), 116.07083 (C5H10NO2+); (*) on in 1st peak
	4.06	342.27521	
	4.13	228.15948	82.06570 (C5H8N+), 128.07069 (C6H10NO2+), 182.15378 (C11H20NO+)
	4.13	257.22238	98.09682 (C6H12N+), 157.13353 (C8H17N2O+)
	4.17	269.22220	100.07610 (C5H10NO+), 169.13351 (C9H17N2O+)
	4.38	230.17513	57.07070 (C4H9+), 74.02430 (C2H4NO2+), 84.08134 (C5H10N+), 88.03981 (C3H6NO2+), 100.11246 (C6H14N+), 130.08630 (C6H12NO2+), 184.16948 (C11H22NO+)
	4.73	264.15961	see growth medium, ES- table
	4.83	244.19083	1st peak: 69.07059 (C5H9+), 88.03982 (C3H6NO2+), 98.09683 (C6H12N+), 116.10723 (C6H14NO+), 144.10191 (C7H14NO2+), 198.18529 (C12H24NO+); 2nd peak: 88.03980 (C3H6NO2+), 144.10188 (C7H14NO2+)
	4.90	632.23187	1st peak: 97.02882 (C5H5O2+), 120.08095 (C8H10N+), 136.06178 (C5H6N5+), 162.04097 (C6H4N5O+), 202.08633 (C12H12NO2+), 220.09691 (C12H14NO3+), 281.09909 (C10H13N6O4+), 316.11795 (C17H18NO5+), 352.13849 (C17H22NO7+); 2nd peak: 120.08097 (C8H10N+), 136.06184 (C5H6N5+), 138.05499 (C7H8NO2+), 156.06543 (C7H10NO3+), 162.04094 (C6H4N5O+), 166.04977 (C8H8NO3+), 184.06036 (C8H10NO4+), 202.08618 (C12H12NO2+), 263.08847 (C10H11N6O3+), 303.13391 (C16H19N2O4+), 321.14447 (C16H21N2O5+), 339.15512 (C16H23N2O6+), 347.12360 (C17H19N2O6+), 500.18936 (C22H26N7O7+)
	5.30	616.23676	see growth medium, ES- table
	5.33	278.17508	105.07018 (C8H9+), 115.05444 (C9H7+), 117.05751 (C8H7N+, rad), 120.08093 (C8H10N+), 130.06517 (C9H8N+), 132.08078 (C9H10N+), 150.09135 (C9H12NO+), 178.08612 (C10H12NO2+)
	6.11	457.19751	see growth medium, ES- table
	6.21	212.23738	
	6.31	280.26367	
	6.52	239.20045	
	6.55	418.27142	
	6.67	590.39038	85.02900 (C4H5O2+)
	6.83	428.30069	
	6.91	314.23239	85.02896 (C4H5O2+), 153.12738 (C10H17O+), 171.13792 (C10H19O2+), 255.15892 (C14H23O4+)
	6.94	356.31610	70.06580 (C4H8N+)
	6.96	310.27396	70.06580 (C4H8N+), 205.15918 (C15H25+), 223.20561 (C15H27O+), 292.26334 (C19H34NO+)
	7.10	324.28943	see comments
	7.26	475.28391	*58.99580 (C2H3S+), *76.02217 (C2H6NS+), *86.99043 (C3H3SO+), *88.02208 (C3H6NS+), *116.01672 (C4H6NSO+), *144.01143 (C5H6NSO2+), *162.02188 (C5H8NSO3+), *179.04823 (C5H11N2SO3+), 261.22104 (C18H29O+), 311.20334 (C18H31SO2+), 319.20923 (C20H31SO+), 337.21948 (C20H33SO2+), 347.20395 (C21H31SO2+), 354.24548 (C20H36NSO2+), 364.23041 (C21H34NSO2+), 365.21454 (C21H33SO3+), 376.22934 (C22H34NSO2+), 394.24167 (C22H36NSO3+), 422.23593 (C23H36NSO4+), 440.24655 (C23H38NSO5+), 457.27328 (C23H41N2SO5+); (*) Cys-Gly and its fragments
	7.34	455.31140	95.06081 (C5H7N2+), 109.07635 (C6H9N2+), 121.07620 (C7H9N2+), 123.09181 (C7H11N2+), 135.09169 (C8H11N2+) and further series of N2 fragments up to C16, 270.22144 (C19H28N+), 287.024802 (C19H31N2+), 305.25858 (C19H33N2O+), 437.30109 (C24H41N2O5+)
	7.39	396.31070	74.02425 (C2H4NO2+), 84.08131 (C5H10N+), 88.03979 (C3H6NO2+), 116.10716 (C6H14NO+), 130.08627 (C6H12NO2+)
	7.66	428.33694	60.08155 (C3H10N+), 85.02894 (C4H5O2+)
	7.72	439.31671	95.06084 (C5H7N2+), 109.07632 (C6H9N2+), 137.07092 (C7H9N2O+), 151.08655 (C8H11N2O+), 223.10779 (C11H15N2O3+), 241.11810 (C11H17N2O4+), 287.24792 (C19H31N2+), 301.26358 (C20H33N2+), 313.26379 (C21H33N2+), 331.27411 (C21H35N2O+), 361.28433 (C22H37N2O2+), 389.27933 (C23H37N2O3+), 403.29550 (C24H39N2O3+), 421.30582 (C24H41N2O4+)
	8.04	339.20660	144.08070 (C10H10N+), 161.10715 (C10H13N2+), 179.10649 (C11H15O2+), 187.08647 (C11H11N2O+), 196.13309 (C11H18NO2+)
	8.27	442.35260	85.02894 (C4H5O2+)
	8.30	301.23721	223.20549 (C15H27O+), 229.19502 (C17H25+), 247.20540 (C17H27O+), 265.21597 (C17H29O2+), 283.22684 (C17H31O3+)

	8.31	426.28476	288.23178 (C19H30NO+), 306.24283 (C19H32NO2+), 318.24274 (C20H32NO2+), 360.25345 (C22H34NO3+), 390.26404 (C23H36NO4+), 408.27460 (C23H38NO5+)
	8.40	285.24234	185.15355 (C11H21O2+), 231.21062 (C17H27+), 249.22116 (C17H29O+), 267.23166 (C17H31O2+)
	8.63	283.22693	205.19508 (C15H25+), 223.20557 (C15H27O+), 229.19501 (C17H25+), 247.20555 (C17H27O+), 265.21603 (C17H29O2+)
	9.02	331.22415	
	9.06	297.24246	219.21074 (C16H27+), 237.22118 (C16H29O+), 243.21059 (C18H27+), 261.22119 (C18H29O+), 279.23172 (C18H31O2+)
ascr	9.21	668.45862	263.27316 (C19H35+), 281.28372 (C19H37O+), 287.27304 (C21H35+), 305.28366 (C21H37O+), 323.29434 (C21H39O2+), 341.30484 (C21H41O3+), 359.31561 (C21H43O4+)
	9.36	476.39493	275.27310 (C20H35+), 293.28369 (C20H37O+), 311.29410 (C20H39O2+), 329.30499 (C20H41O3+)
	9.38	211.20580	
	9.42	457.36377	2nd peak: *87.05579 (C3H7N2O+), *88.03979 (C3H6NO2+), *133.06075 (C4H9N2O3+), 394.33167 (C24H44NO3+), 422.32617 (C25H44NO4+), 439.35263 (C25H47N2O4+); (*) Asn and its fragments
ascr	9.47	483.32962	353.26608 (C19H38O4Na+)
	9.47	313.27374	199.16934 (C12H23O2+), 213.18494 (C13H25O2+), 277.25229 (C19H33O+), 295.26276 (C19H35O2+)
	9.49	287.25790	7.95 and 8.10 min: 233.22609 (C17H29+), 251.23662 (C17H31O+); 8.84 min: maynot be diff. based on 269.24750; 9.49 min: 233.22618 (C17H29+), 251.23653 (C17H31O+), 269.24722 (C17H33O2+)
	9.49	309.24005	
	9.54	227.20062	191.17937 (C14H23+)
S	9.56	388.28793	75.02692 (C3H7S+), 92.05330 (C3H10NS+), 219.21069 (C16H27+), 243.21051 (C18H27+), 261.22113 (C18H29O+), 304.26331 (C20H34NO+), 322.27380 (C20H36NO2+), 352.26666 (C21H38NSO+), 370.27725 (C21H40NSO2+)
	9.56	307.22427	
	9.57	333.23987	
	9.61	583.49659	
	9.65	223.20564	
	9.66	682.47375	see growth medium, ES- table
	9.94	255.23177	219.21059 (C16H27+), 237.22107 (C16H29O+)
	9.98	708.48975	see growth medium, ES- table
	10.01	458.38403	1st peak: *86.09698 (C5H12N+), *132.10196 (C6H14NO2+), 309.27863 (C20H37O2+), (*) Leu/Ile and its fragment; 2nd peak: **72.08142 (C4H10N+), **118.08641 (C5H12NO2+), 305.28314 (C21H37O+), 323.29419 (C21H39O2+), (**) Val and its fragment
	10.02	327.28928	213.18472 (C13H25O2+), 227.20042 (C14H27O2+), 291.26801 (C20H35O+), 309.27856 (C20H37O2+)
	10.18	696.48914	see growth medium, ES- table
	10.24	295.22650	2nd peak: 217.19507 (C16H25+), 235.20557 (C16H27O+), 245.18993 (C17H25O+), 277.21588 (C18H29O2+)
	10.25	237.22107	
	10.43	305.24741	
	10.43	487.39969	303.30484 (C22H39+), 321.31509 (C22H41O+)
	10.50	665.41718	
	10.52	259.26318	
	10.54	275.23685	
	10.56	386.36292	2nd (larger) peak: 269.24734 (C17H33O2+), 333.31503 (C23H41O+), 351.32556 (C23H43O2+)
	10.56	472.39972	86.09695 (C5H12N+), 132.10193 (C6H14NO2+), 323.28422 (C21H39O2+)
	10.58	506.40527	see growth medium, ES- table
	10.58	471.37943	1st peak: 83.06091 (C4H7N2+), 84.04494 (C4H6NO+), **129.06595 (C5H9N2O2+), **130.04993 (C5H8NO3+), **147.07635 (C5H11N2O3+), 299.25815 (C18H35O3+), 453.36816 (C26H49N2O4+), (**) Gln and its fragments; 2nd peak: *87.05583 (C3H7N2O+), *88.03983 (C3H6NO2+), *133.06085 (C4H9N2O3+), 408.34723 (C25H46NO3+), 436.34235 (C26H46NO4+), 453.36960 (C26H49N2O4+); (*) Asn and its fragments
	10.58	710.50494	see growth medium, ES- table
ascr	10.60	652.46326	*85.02892 (C4H5O2+), *97.02877 (C5H5O2+), *113.05994 (C6H9O2+), *127.03899 (C6H7O3+), *145.04950 (C6H9O4+), 289.28839 (C21H37+), 307.29959 (C21H39O+), 325.31000 (C21H41O2+); (*) glucose fragments
	10.63	476.35864	62.06079 (C2H8NO+), 297.27911 (C19H37O2+), 314.30508 (C19H40NO2+)
	10.75	334.27405	110.06033 (C6H8NO+), 111.06813 (C6H9NO+, rad), 124.07579 (C7H10NO+), 304.26321 (C20H34NO+)
	10.79	251.23682	
ascr	10.92	622.45288	see growth medium, ES- table
	11.06	501.41519	317.32004 (C23H41+), 335.33054 (C23H43O+), 353.34082 (C23H45O2+)
	11.06	629.47437	1st peak: 83.06097 (C4H7N2+), 84.04498 (C4H6NO+), 101.07135 (C4H9N2O+), 129.06596 (C5H9N2O2+), 130.04994 (C5H8NO3+), 147.07637 (C5H11N2O3+), 335.33069 (C23H43O+), 464.37433 (C28H50NO4+), 481.40012 (C28H53N2O4+), 499.40958 (C28H55N2O5+); 2nd and 3rd peaks: 87.05583 (C3H7N2O+), 88.03983 (C3H6NO2+), 116.03453 (C4H6NO3+), 133.06078 (C4H9N2O3+), 349.34616 (C24H45O+), 436.37772 (C27H50NO3+), 464.37372 (C28H50NO4+), 481.39999 (C28H53N2O4+), 499.41113 (C28H55N2O5+)
	11.08	395.35223	
	11.11	486.41544	1st and 2nd peaks: 86.09697 (C5H12N+), 132.10196 (C6H14NO2+), 337.31006 (C22H41O2+); 3rd peak: 72.08147 (C4H10N+), 118.08649 (C5H12NO2+), 351.32550 (C23H43O2+)
ascr	11.13	503.39465	see growth medium, ES- table

	11.14	355.32062	241.21585 (C15H29O2+), 255.23161 (C16H31O2+), 319.29929 (C22H39O+), 337.30957 (C22H41O2+)
ascr	11.14	666.47919	see growth medium, ES- table
	11.20	373.33142	277.28873 (C20H37+), 295.29941 (C20H39O+), 301.28897 (C22H37+), 319.29922 (C22H39O+)
	11.26	424.37860	141.12735 (C9H17O+), 406.36765 (C26H48NO2+)
	11.38	643.49011	see growth medium, ES- table
	11.52	383.35205	1st peak is a fragment of 545.40497/675.46814/692.49469; 2nd peak: 269.24753 (C17H33O2+), 283.26294 (C18H35O2+), 329.32053 (C24H41+), 347.33075 (C24H43O+), 365.34122 (C24H45O2+)
ascr	11.55	692.49469	see growth medium, ES- table
	11.56	369.33624	1st peak: 255.23184 (C16H31O2+), 269.24744 (C17H33O2+), 333.31528 (C23H41O+), 351.32574 (C23H43O2+); 2nd peak: 291.30457 (C21H39+), 309.31516 (C21H41O+), 315.30472 (C23H39+), 333.31479 (C23H41O+), 351.32501 (C23H43O2+)
	11.59	565.40063	130.06526 (C9H8N+), 132.04446 (C8H6NO+), 145.07610 (C9H9N2+), 173.07098 (C10H9N2O+), 201.10231 (C12H13N2O+), 244.13321 (C15H18NO2+), 519.39490 (C34H51N2O2+), 547.38953 (C35H51N2O3+)
ascr	11.67	534.43719	see growth medium, ES- table
	11.67	387.34708	291.30429 (C21H39+), 309.31503 (C21H41O+), 315.30444 (C23H39+), 333.31461 (C23H41O+)
	11.68	680.49506	85.02897 (C4H5O2+), 97.02881 (C5H5O2+), 113.06000 (C6H9O2+), 127.03908 (C6H7O3+), 145.04958 (C6H9O4+), 317.32047 (C23H41+), 335.33081 (C23H43O+), 353.34143 (C23H45O2+)
	11.68	567.38733	see growth medium, ES- table
	11.75	446.38434	263.27313 (C19H35+), 281.28372 (C19H37O+)
	11.76	385.36768	331.33572 (C24H43+), 349.34641 (C24H45O+)
	11.83	694.51080	see growth medium, ES- table
	12.08	401.36282	1st and 2nd peaks: 291.30478 (C21H39+), 309.31613 (C21H41O+), 329.32022 (C24H41+), 347.33069 (C24H43O+); 3rd peak: 329.32022 (C24H41+), 347.33069 (C24H43O+)
	12.13	548.45288	see 529.41119 at 10.79 min in growth medium, ES- table
	12.27	641.46100	
ascr	12.28	460.40009	277.28912 (C20H37+), 295.29941 (C20H39O+), 313.30991 (C20H41O2+, only in 2nd peak)
ascr	12.32	664.50043	85.02897 (C4H5O2+), 97.02885 (C5H5O2+), 113.06002 (C6H9O2+), 127.03912 (C6H7O3+), 145.04959 (C6H9O4+), 319.33609 (C23H43+), 337.34634 (C23H45O+)
ascr	12.56	720.52612	see growth medium, ES- table
	12.56	411.38327	319.33582 (C23H43+), 347.36755 (C25H47+), 357.35129 (C26H45+), 375.36182 (C26H47O+)
ascr	12.63	516.42645	315.30453 (C23H39+), 333.31488 (C23H41O+), 351.32532 (C23H43O2+)
ascr	12.75	562.46753	319.33572 (C23H43+), 337.34616 (C23H45O+), 343.33557 (C25H43+), 361.34607 (C25H45O+), 379.35681 (C25H47O2+), 397.36749 (C25H49O3+)
ascr	12.77	474.41571	291.30441 (C21H39+), 309.31497 (C21H41O+)
ascr	12.80	722.54144	see growth medium, ES- table
	12.81	609.43365	
ascr	12.99	606.49457	331.33591 (C24H43+), 349.34637 (C24H45O+), 367.35715 (C24H47O2+), 423.38321 (C27H51O3+), 441.39398 (C27H53O4+)
ascr	13.06	371.35159	see growth medium, ES- table
	13.13	581.43903	
ascr	13.25	488.43115	305.32007 (C22H41+), 323.33057 (C22H43O+)
ascr	13.71	595.45496	see growth medium, ES- table
ascr	13.74	502.44705	319.33566 (C23H43+), 337.34619 (C23H45O+)
	13.79	637.46527	
ascr	14.14	516.46271	333.35144 (C24H45+), 351.36203 (C24H47O+)

Table S18. SMID-DB identifiers, retention times, and *m/z* of known ascarosides detected in the analyzed *C. elegans* N2 and *P. pacificus* RS2333 cultures. For all ascarosides except ascr#4, *m/z* corresponds to molecular ions, $[M-H]^-$. For ascr#4, listed *m/z* is for the formic acid (FA) adduct, $[M+FA-H]^-$.

SMID-DB ID	RT (min)	*m/z* calc. (ES-)	Species
ascr#5	1.64	219.08741	Cel
ascr#11	2.89	233.10306	Cel
ascr#9	3.59	247.11871	Cel, Ppa
oscr#9	3.68	247.11871	Cel
ascr#12	4.15	261.13436	Cel, Ppa
ascr#7	4.49	273.13436	Cel
ascr#1	4.68	275.15001	Cel, Ppa
ascr#14	5.22	289.16566	Cel
ascr#3	5.56	301.16566	Cel
ascr#10	5.76	303.18131	Cel
ascr#16	6.29	317.19696	Cel
ascr#18	6.82	331.21261	Cel
ascr#20	7.35	345.22826	Cel
ascr#22	7.88	359.24391	Cel
icas#9	6.56	390.15583	Cel
icas#3	7.89	444.20278	Cel
icas#10	8.07	446.21843	Cel
osas#9	4.91	482.20317	Cel
tsas#9	5.52	466.20826	Cel
osas#10	6.48	538.26577	Cel
ascr#4 (+FA)	3.93	453.19775	Cel
osas#2	5.39	480.22391	Cel
icas#7	7.12	416.17148	Cel
icas#1	7.23	418.18713	Cel
pasc#9	5.65	466.20826	Ppa
pasc#12	5.92	480.22391	Ppa
pasc#1	6.21	494.23956	Ppa
ubas#1	5.88	605.29271	Ppa
ubas#2	6.1	619.30836	Ppa
dasc#1	6.6	533.29674	Ppa
part#9	3.75	247.11871	Ppa
npar#1	4.55	641.24241	Ppa
npar#2	4.76	509.20015	Ppa
npar#3	4.71	525.19506	Ppa
pasa#9	6.8	585.24537	Ppa

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