

Table S1 The physical behavioral observations of *E. diaphana* after two weeks compared to the control group.

Physical and Behavioral Observations	3 ppb	10 ppb	30 ppb	50 ppb	70 ppb	90 ppb
Bleaching	No	No	No	Slight	Slight	Slight
Tentacles	Negligible	Slightly disheveled	Disheveled	Disheveled	Disheveled	Significantly disheveled
Sluggish Reactions	Negligible	Slightly reduced	Reduced	Significantly reduced	Significantly reduced	Significantly reduced

Table S2 The metabolites with p values and fold change under various concentrations of atrazine treatment. Fold Change (FC)

Metabolites	3 ppb vs control		10 ppb vs control		30 ppb vs control		50 ppb vs control		70 ppb vs control		90 ppb vs control	
	p values	Fold Change	p values	Fold Change	p values	Fold Change	p values	Fold Change	p values	Fold Change	p values	Fold Change
2-Oxocaproate	3.92E-01	0.93	3.89E-01	0.94	1.50E-01	0.90	1.95E-01	0.91	1.10E-01	0.89	7.16E-02	0.83
4-Aminobutyrate	4.88E-01	1.15	1.92E-01	1.21	5.60E-01	0.93	8.69E-01	0.98	8.87E-01	0.98	4.62E-01	0.91
Acetate	7.80E-01	1.03	8.86E-01	0.99	5.74E-02	0.86	5.46E-02	0.87	1.71E-01	0.88	1.25E-01	0.86
Adenosine	1.99E-01	1.34	7.87E-01	0.99	5.65E-01	1.11	6.12E-01	1.19	9.60E-02	1.42	1.04E-01	1.63
Alanine	1.83E-01	0.94	8.54E-02	0.93	1.82E-02	0.90	4.23E-03	0.88	7.75E-03	0.86	1.29E-02	0.87
Aspartate	5.97E-01	0.94	1.87E-01	1.16	8.82E-01	1.01	4.59E-01	0.91	8.75E-01	0.97	6.69E-01	0.95
Betaine	4.16E-01	0.98	2.86E-01	0.96	3.15E-01	0.98	1.96E-01	0.96	2.50E-02	0.95	4.48E-01	0.98
Choline	6.81E-01	0.97	1.04E-01	1.18	6.79E-01	1.02	4.09E-01	0.94	3.56E-01	1.09	4.45E-01	1.08

Citrate	1.92E-01	1.19	1.71E-02	1.28	1.04E-01	1.24	1.41E-01	1.18	5.29E-02	1.23	4.46E-01	1.14
Creatine	6.79E-02	1.11	7.48E-02	1.11	2.80E-01	1.06	9.06E-01	1.01	1.53E-01	1.10	9.98E-01	1.02
Creatinine	1.40E-01	1.14	1.57E-01	1.11	2.25E-01	1.12	8.87E-01	1.03	1.95E-01	1.13	8.57E-01	1.03
Cytidine	1.11E-01	2.33	2.46E-01	1.42	1.92E-01	2.03	8.72E-01	1.39	1.09E-01	2.37	1.38E-01	2.32
dCTP	2.13E-01	1.25	6.38E-01	0.93	1.09E-02	1.46	4.15E-03	1.94	8.54E-03	1.76	2.96E-01	1.27
Dimethyl sulfone	8.97E-01	1.02	5.22E-01	1.06	8.09E-01	1.09	5.68E-01	0.98	3.39E-01	1.16	8.75E-01	1.03
Ethanol	2.58E-01	1.36	4.93E-01	1.09	1.80E-01	1.43	7.93E-01	1.28	9.28E-02	1.59	3.71E-01	1.44
Formate	4.74E-01	1.18	3.26E-01	1.11	2.35E-01	1.24	2.35E-01	1.24	1.27E-01	1.49	1.53E-01	1.62
Glucose	1.17E-01	0.91	4.87E-02	0.89	7.96E-01	0.98	6.03E-01	1.03	4.39E-02	0.85	2.04E-02	0.85
Glutamate	3.26E-02	1.18	2.90E-01	1.08	7.47E-03	1.21	6.85E-03	1.18	3.70E-04	1.29	2.55E-04	1.32
Glutamine	6.62E-02	1.22	4.15E-02	1.19	8.87E-01	1.00	7.31E-02	1.12	4.75E-03	1.26	9.52E-02	1.31
Glycine	5.91E-01	1.03	1.40E-01	0.93	4.62E-01	0.96	8.50E-01	0.99	1.88E-01	0.91	7.79E-02	0.88
Guanosine	8.59E-01	1.03	6.53E-01	1.05	6.56E-02	0.92	3.58E-02	1.16	5.07E-01	0.96	4.03E-01	0.95
Histidine	7.03E-02	1.19	2.32E-01	1.16	1.84E-01	1.15	3.22E-01	1.17	4.35E-02	1.22	4.99E-01	1.14
Homoserine	4.17E-01	1.04	7.00E-01	0.98	5.07E-01	1.04	2.88E-01	1.06	9.16E-01	0.99	1.66E-01	1.08
Hydroxyacetone	3.02E-01	1.10	1.57E-01	1.11	4.27E-01	1.10	1.03E-01	1.16	2.45E-02	1.23	6.44E-02	1.23
Hypoxanthine	8.80E-02	1.31	3.09E-01	1.14	2.83E-01	1.25	9.33E-01	1.03	1.32E-01	1.28	1.34E-01	1.24

IMP	9.20E-01	0.98	9.45E-01	0.98	6.74E-01	1.03	7.41E-01	1.10	6.74E-01	1.03	6.48E-01	1.08
Inosine	7.90E-01	0.98	9.19E-01	0.99	3.63E-01	0.94	9.86E-01	1.01	7.20E-01	1.02	2.14E-01	1.11
Isoleucine	7.81E-02	1.14	1.90E-01	1.23	4.37E-01	1.09	2.94E-01	1.12	1.08E-02	1.30	1.82E-01	1.13
Lactate	8.66E-01	1.03	7.23E-01	1.04	1.36E-01	1.13	6.62E-01	1.06	8.61E-02	1.17	5.94E-03	1.28
Leucine	1.28E-01	1.11	8.10E-01	1.04	4.22E-01	1.08	1.98E-01	1.11	2.56E-02	1.21	1.39E-01	1.14
Lysine	1.48E-01	1.08	1.00E+00	1.00	3.80E-01	1.04	3.69E-01	1.04	7.49E-02	1.09	3.11E-01	1.09
Malate	9.98E-01	1.00	8.13E-01	1.03	9.85E-01	1.00	3.93E-01	0.89	6.11E-01	0.94	8.60E-01	0.98
Methanol	9.78E-01	1.03	7.27E-01	0.95	2.96E-01	1.16	9.12E-01	0.99	2.34E-01	1.62	1.21E-01	1.42
Methionine	7.39E-02	1.13	1.14E-01	1.10	4.23E-01	1.07	8.65E-02	1.12	3.57E-02	1.16	3.36E-02	1.19
myo-Inositol	2.56E-01	0.92	7.97E-02	0.89	5.37E-01	0.96	7.84E-01	1.01	1.13E-02	0.77	1.04E-02	0.79
O-Phosphocholine	8.47E-01	1.02	3.37E-01	1.06	1.19E-01	1.08	7.01E-01	1.05	4.90E-01	1.04	7.18E-01	0.98
Phenylalanine	2.97E-02	1.21	2.19E-01	1.13	5.20E-01	1.08	3.13E-01	1.11	5.79E-02	1.24	5.32E-01	1.12
Serine	3.68E-01	0.93	5.74E-01	0.96	2.61E-01	0.92	9.53E-01	1.00	1.14E-01	0.87	1.51E-01	0.88
sn-Glycero-3-phosphocholine	8.39E-01	0.99	2.87E-01	1.14	5.33E-01	1.05	3.15E-01	0.89	7.73E-01	1.01	8.13E-01	1.02
Succinate	2.03E-01	0.92	4.75E-01	0.95	1.57E-02	0.82	1.82E-01	0.90	9.28E-02	0.89	2.56E-02	0.84
Taurine	1.53E-01	0.95	6.68E-01	1.01	2.05E-01	0.95	1.91E-01	0.94	5.58E-03	0.91	3.62E-01	0.95
Thymidine	1.02E-01	1.55	3.87E-01	1.17	2.98E-01	1.29	4.89E-01	1.21	7.33E-02	1.62	1.25E-01	1.61

Trimethylamine	1.80E-01	0.81	8.11E-02	0.75	1.55E-02	0.74	1.77E-01	0.85	8.13E-02	0.74	2.13E-02	0.65
Tyrosine	1.66E-01	1.20	5.36E-01	1.11	3.38E-01	0.87	7.27E-01	1.04	3.92E-01	1.18	6.89E-01	1.15
Valine	5.83E-02	1.12	8.49E-01	1.02	5.45E-01	1.05	1.63E-01	1.09	8.94E-02	1.11	2.17E-01	1.10
Xylose	1.82E-01	0.85	4.13E-01	0.93	2.91E-01	0.89	7.74E-02	1.18	2.55E-01	0.88	3.07E-01	0.89
β -Alanine	8.47E-02	1.22	2.29E-02	1.27	7.07E-02	1.19	1.03E-01	1.19	1.88E-02	1.29	7.28E-03	1.43

Table S3 The detailed metabolites assignment, the number is corresponding to **Figure S1**.

Number	Metabolites	Chemical shift (ppm)	Pattern	Confidence	notation
1	TSP	0.00	reference	High	
2	Isoleucine	0.94	triplet	High	
3	Leucine	0.95	triplet	High	
4	Valine	0.99	doublet	High	
		1.04	doublet	High	
5	Ethanol	1.16	triplet	High	
6	Lactate	1.32	doublet	High	
7	Alanine	1.47	doublet	High	
8	Lysine	1.74	multiplet	High	
		3.06	triplet	High	
9	Acetate	1.93	singlet	High	
10	Glutamate	2.02	multiplet	High	
		2.36	multiplet	High	
11	Methionine	2.17	multiplet	High	
		2.65	triplet	High	
12	Hydroxyacetone	2.21	singlet	Medium	
	Hydroxyacetone	4.37	singlet	Medium	
13	4-Aminobutyrate	2.30	triplet	High	
14	Succinate	2.41	singlet	High	
15	Glutamine	2.45	multiplet	High	
16	Citrate	2.53	multiplet	High	
17	Malate	2.69	doublet	Medium	Overlap
18	2-Oxocaproate	2.73	triplet	High	

19	Aspartate	2.83	doublet	High	
20	Trimethylamine	2.93	singlet	Medium	
21	Creatine	3.04	singlet	Medium	Overlap
22	Creatinine	3.06	singlet	Medium	Overlap
23	Dimethyl sulfone	3.15	singlet	Medium	
24	Choline	3.20	singlet	Medium	
25	O-Phosphocholine	3.23	singlet	Medium	
26	sn-Glycero-3-phosphocholine	3.24	singlet	Medium	
27	Betaine	3.27	singlet	High	
		3.91	singlet	High	
28	Methanol	3.36	singlet	High	
29	Taurine	3.42	triplet	High	
30	myo-Inositol	3.56	doublet	Medium	
		3.65	doublet		
31	Glycine	3.58	singlet	High	
32	Glucose	3.70	multiplet	High	
		4.65	doublet		
33	Homoserine	3.77	multiplet	Medium	
34	Serine	3.96	multiplet	High	
35	Adenosine	8.34	singlet	Medium	
36	Xylose	4.60	doublet	High	
37	Cytidine	7.85	doublet	Medium	
38	Guanosine	5.92	doublet	Medium	
39	dctp	6.15	doublet	Medium	
40	Tyrosine	6.93	multiplet	High	
41	Histidine	7.87	singlet	Medium	
42	Phenylalanine	7.38	multiplet	High	
43	Thymidine	7.64	doublet	High	
44	Hypoxanthine	8.21	singlet	High	
		8.22	singlet		

45	Inosine	8.26	singlet	Medium	
46	Formate	8.46	singlet	Medium	
47	IMP	8.56	singlet	Medium	
48	β -Alanine*	2.59	triplet	Medium	

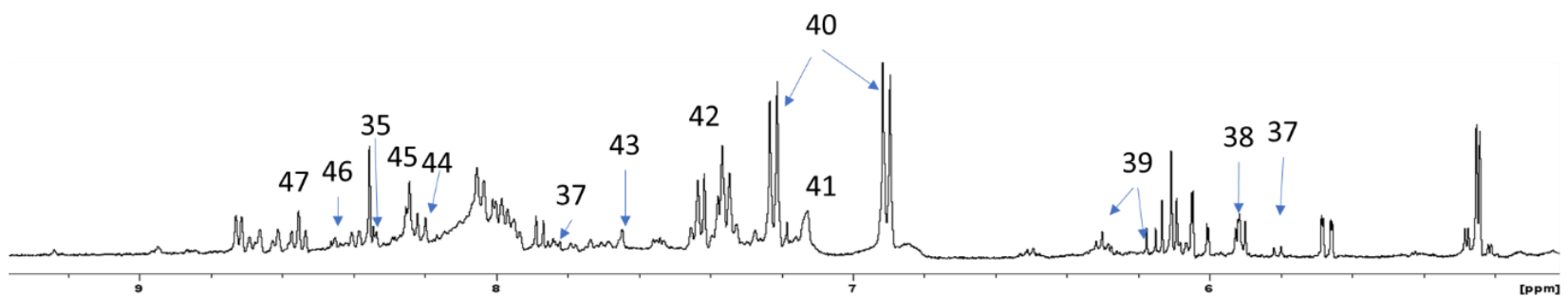
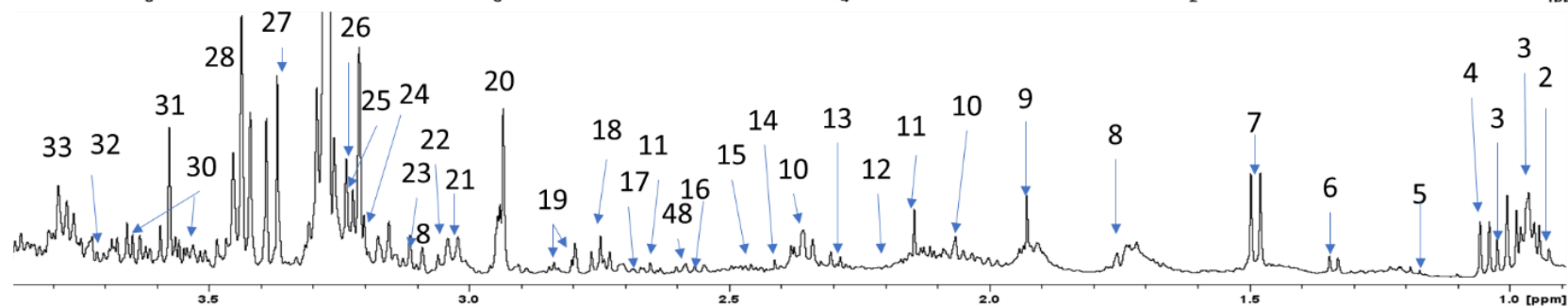
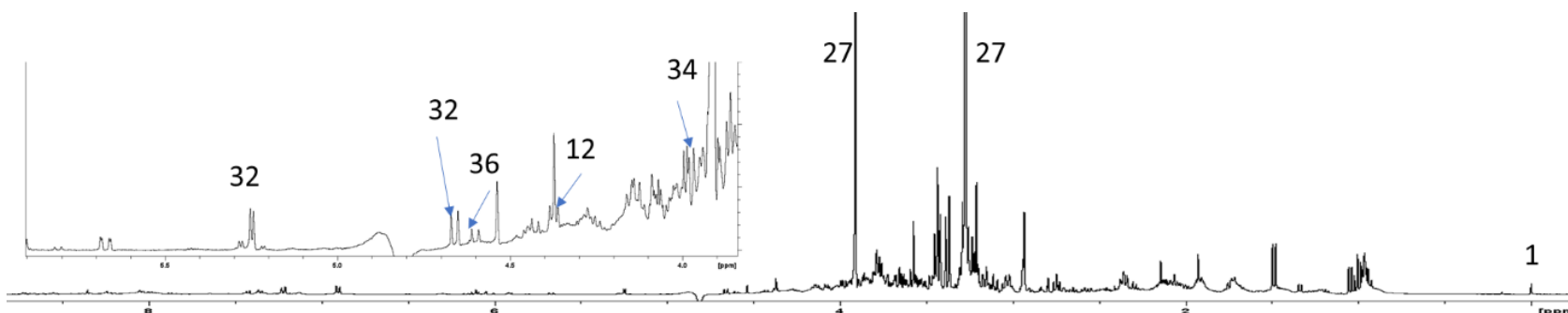


Figure S1 Representative spectrum of the metabolites.

1,TSP (reference), 2,Isoleucine, 3,Leucine, 4,Valine, 5,Ethanol, 6,Lactate, 7,Alanine, 8,Lysine, 9,Acetate, 10,Glutamate, 11,Methionine, 12,Hydroxyacetone, 13,4-Aminobutyrate, 14,Succinate, 15,Glutamine, 16,Citrate, 17,Malate, 18,2-Oxocaproate, 19,Aspartate, 20,Trimethylamine, 21,Creatine, 22,Creatinine, 23,Dimethyl sulfone, 24,Choline, 25,o-Phosphocholine, 26,sn-Glycero-3-phosphocholine, 27,Betaine, 28,Methanol, 29,Taurine, 30,myo-Inositol, 31,Glycine, 32,Glucose, 33,Homoserine, 34,Serine, 35,Adenosine, 36,Xylose, 37,Cytidine, 38,Guanosine, 39,dctp, 40,Tyrosine, 41,Histidine, 42,Phenylalanine, 43,Thymidine, 44,Hypoxanthine, 45,Inosine, 46,Formate, 47,IMP, 48, β -Alanine.

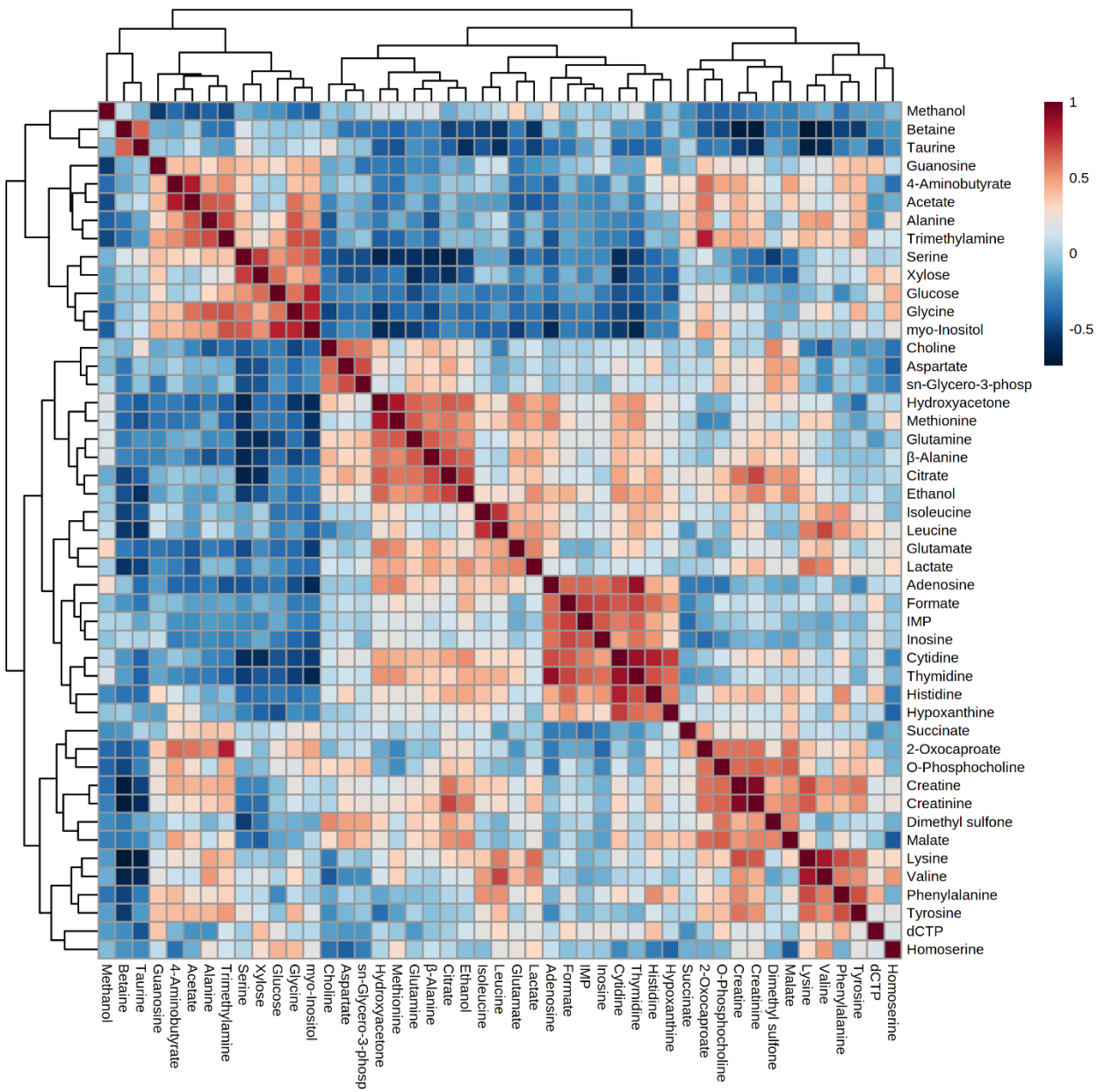


Figure S2 The correlation relationship heatmap of the metabolites. Pearson correlations were applied for the heatmap.