Supporting Information

Cover sheet

Title	Potential role of methanogens in microbial reductive dechlorination of organic chlorinated pollutants in situ
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1. Organic chlorinated pollutants (OCPs)

Table S1 Concentrations of various OCPs worldwide

Ref.	Year	Type	Site	OCPs	Ref.
1	2008	River	Yalu River	OCPs 34.62 ng g^{-1} dw^{-1}	Xie et al., 2017 (1)
2	2008	River	Shuang Long River	OCPs 355.09 ng g^{-1} dw^{-1}	
3	2008	River	Luanhe River	OCPs 11.87 ng g^{-1} dw^{-1}	
4	2008	River	Daling River	OCPs 86.40 ng g^{-1} dw^{-1}	
5	2008	River	Bohai Sea	OCPs 86.94 ng g^{-1} dw^{-1}	
6	2008-2011	River	Daling River estuary	DDTs 6.83 ng g^{-1} dw^{-1}	Guo et al., 2015 (2)
7	2013	River	Po River Prodelta	PCBs 18.72 ng hr^{-1}	Quero et al., 2015 (3)
8	2013	River	Mar Piccolo of Taranto	PCBs 466.72 ng hr^{-1}	
9	<2016	Upland	Copenhagen	OCPs 0.70 ng g^{-1} dw^{-1}	Feld et al., 2016 (4)
10	2011	Wastewater lagoon	Altavista, America	PCB 1.47 g kg^{-1}	Mattes et al., 2018(5)
11	2006	Valley glacier	Jamtalferner	PCBs 799.22 pg g^{-1} dry weight	Weiland-Brauer et al., 2017 (6)
12	2014-2015	Greenhouse soils	China	OCPs 136 ng g^{-1}	Sun et al., 2018 (7)
13	2014-2015	Open fields	China	OCPs 77.2 ng g^{-1}	
14	2011	Sediment	Chinhat village, India	HCHs 0.60 mg kg^{-1}	Negi et al., 2017 (8)
15	2013	Arable soils	China	DDTs 1.08 ng g^{-1} dw^{-1}	Niu et al., 2016 (9)
16	2015	Monitoring Wells	Hawaii, America	PCE 49 μg L^{-1}	Liang et al., 2017 (10)
17	2013	Farmlands	China	HCHs 2.302 ng g^{-1}	Xu et al., 2018 (11)
18	<2018	Agricultural soil	Ningbo, China	OCPs 4.51 mg kg^{-1}	Ali et al., 2019 (12)
19	2013	Paddy	Changxing, China	Atrazine 73.85 mg kg^{-1}	Ma et al., 2017 (13)
20	2013	Groundwater and stream water	Wonju, Korea	TCE 448.6 μg L^{-1} *cis*-DCE 81.3μg L^{-1} VC 4.33 μg L^{-1}	Lee et al., 2015 (14)
21	<2018	Abandoned insecticide plant	Wuhan, China	HCHs 1.44 mg kg^{-1} DDTs 1.33 mg kg^{-1} γ-HCH 0.1342 mg kg^{-1}	Sun et al., 2019 (15)
22	<2017	Groundwater	China	δ-HCH 82.21 μg L^{-1}	Pirsaheb et al., 2017 (16)

23	<2017	Surface water	Iran	Diazinon 768.91 μg L^{-1}	
24	2000-2009	Mangrove sediment	Singapore, Vietnam, China, India, Tanzania, Senegal, Brazil, Costa Rica	PCBs 0.3 - 184.16 ng g^{-1} dw^{-1}	Bayen et al., 2012 (17)

11 Organic chlorinated pollutants (OCPs); Dichloro-diphenyl-trichloroethane (DDT);
12 Hexachlorocyclohexanes (HCHs); Polychlorinated biphenyls (PCBs); Tetrachloroethene (PCE);
13 Dichloroethane (DCE); Vinyl chloride (VC).
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2 Methods

2.1 Meta-analysis of CH_4 production

Table S2. List of publications of meta1

No.	Locations	System	Pollutants	Concentration (ppm)	Reference
1	20.46 N 85.92 E	Paddy	HCHs	14.88, 18, 18.6	Satpathy et al., 1997 (18)
2	28.25 N 116.92 E	Paddy	DDTs	33.28	Liu et al., 2016 (19)
3	51.35 N 12.43 E	Culture	HCHs	5, 50, 150, 183.02	Lian et al., 2018 (20)
4	28.25 N 116.92 E	Paddy	HCB	1.82	Liu et al., 2010 (21)
5	28.25 N 116.92 E	Paddy	HCB	0.88	Liu et al., 2010 (22)
6	48.49 N 11.44 E	Soil	HCB	445.22	Brahushi et al., 2004 (23)
7	38.03 N 84.50 W	Paddy	PCP	75	Meade et al., 2005 (24)
8	40.55 N 3.69 W	Sludge	PCP	20, 50, 100	Puyol et al., 2012 (25)
9	35.00 N 136.58 E	Paddy	PCP	15.98	Li et al., 2010 (26)
10	35.16 N 136.97 E	Paddy	PCP	11.98, 13.32	Li et al., 2010 (27)
11	45.49 N 73.67 W	Sludge	PCP	100	Tartakovsky et al., 2000 (28)
12	40.22 N 116.25 E	Sludge	PCP	14.9	Xue et al., 2013 (29)
13	21.99 S 47.92 W	Sludge	PCP	10	Baraldi et al., 2008 (30)
14	46.73 N 117.01 W	Sludge	PCP	50	Kamashwaran et al., 2001 (31)
15	22.03 N 112.79 E	Paddy	PCP	8	Tong et al., 2015 (32)
16	28.63 N 77.22 E	Sludge	PCP	100, 200, 300	Khan et al., 2017 (33)
17	25.09 N 121.55 E	Soil	PCP	10	Chang et al., 1996 (34)
18	42.69 N 84.50 W	Sludge	PCP	1, 2.5	Wu et al., 1993 (35)
19	45.77 N 4.69 W	Soil	PCE	160	David et al., 2015 (36)
20	51.50 N 0.18 W	Wastewater	PCE	10	Ohandja et al., 2009 (37)
21	42.06 N 87.68	Sludge	3-chlorobenzoate	36.8	Becker et al., 2005 (38)

	W				
22	44.98 N 93.23 W	Culture	PCE	1.10	Muenzner et al., 2002 (39)
23	43.52 N 112.05 W	Groundwater	TCE	0.005	Conrad et al., 2010 (40)
24	45.49 N 73.67 W	Sludge	PCE	50	Guiot et al., 2008 (41)
25	22.75 N 120.28 E	Culture	Tetrachloride	30	Lien et al., 2007 (42)
26	23.56 S 46.73 W	Sludge	PCBs	0.0002	de Lima et al., 2018 (43)
27	50.82 N 19.11 E	Sludge	PCBs	23.4	Rosinska et al., 2017 (44)
28	44.49 N 11.33 E	Culture	PCBs	1	Nuzzo et al., 2017 (45)
29	23.56 S 46.73 W	Sludge	PCBs	0.5, 1.5, 3, 4.5, 6	de Lima et al., 2016 (46)
30	39.89 N 32.78 E	Sludge	PCBs	1, 10, 20, 30	Kaya et al., 2013 (47)
31	0.7 N 37.22 E 0.08 N 35.13 E	Paddy	DDTs	30	Kengara et al., 2019 (48)
32	54.85 N 83.11 E	Culture	CH_2Cl_2	3880	Stoyanov et al., 2018 (49)
33	49.27 N 123.25 W	Groundwater	TCE	1443	Chong et al., 2017(50)
34	31.02 N 121.43 E	Groundwater	TCA	2.88	Wang et al., 2017 (51)
35	43.66 N 79.39 W	Culture	Chlorobenzene	56.5	Liang et al., 2013 (52)
36	45.74 N 126.73 E	Sludge	TCE	36.5	Zhang et al., 2015 (53)

Hexachlorocyclohexanes (HCHs); Dichlorodiphenyltrichloroethanes (DDTs); Hexachlorobenzene (HCB); Pentachlorophenol (PCP); Short-chain chlorinated organics (Short-chain), including tetrachloroethylene (PCE), trichloroethene (TCE), vinyl chloride (VC), etc.; Polychlorinated biphenyls (PCBs); Trichloroethane (TCA).

2.2 Meta-analysis of microbial communities

The raw sequence data were downloaded from the National Center for Biotechnology Information (NCBI, https://www.ncbi.nlm.nih.gov). The key words were OCPs (chlorinated, organochlorine, DDT, HCHs, HCB, PCP, TCE, PCBs, etc.) and microbes (microbial, primer, 16S, and Illumina, etc.).

Table S3. List of meta2

No.	Locations	System	Primer	Pollutants	Concentration (ppm)	Reference
1	30.84 N 110.72 E	Paddy	520F/802R	PCP	39.95	Xu et al., 2018 (54)
2	21.82 N 112.46 E	Soil	520F/802R	PCP	40	Cheng et al., 2019 (55)
3	21.82 N 112.46 E	Soil	520F/807R	PCP	19.97	Xu et al., 2017 (56)
4	28.25 N 116.92 E	Paddy	338F/806R	HCB	3	Song et al., 2017 (57)
5	31.28 N 121.50 E	Sediment	mcrA dsrA	Chloroform	35-70	Chen et al., 2015 (58)
6	22.26 N 112.87 E	Paddy	515F/806R	PCP	4.79	Chen et al., 2018(59)
7	41.19 N 121.38 E	Sediment	410F/658R	HCHs, DDTs	0.43	Guo et al., 2015 (2)
8	23.35 N 113.19 E	Soil	515F/806R	PCBs	1.22	Jiang et al., 2018 (60)
9	42.99 N 82.30 W	Groundwater	926F/1392R	Chlorinated ethenes	0.8291	Kocur et al.., 2016 (61)

10	44.99 N 12.54 E	Sediment	341F/785 R	PAHs & PCBs	0.00005	Quero et al., 2015 (3)
11	55.36 N 12.09 E	Groundwater	341F/806 R	DCPP, MCPP, and 4-CPP	1.20	Feld et al., 2016 (4)
12	40.67 N 89.68 W	Culture	515F/806 R	Atrazine	20	Muturi et al., 2017 (62)
13	27.13 N 120.26 E	Groundwater	27R/534 R	PCE, TCE	1	Kao et al., 2016 (63)
14	45.74 N 126.73 E	Sludge	341F/806 R	TCE	36.50	Zhang et al., 2015 (53)
15	41.74 N 111.87 W	Groundwater	515F/907 R	TCE	10	Mirza et al., 2017 (64)
16	29.97 N 113.68 E	Soil	27F/538R	HCHs, DDTs	20	Sun et al., 2015 (65)
17	32.27 N 118.76 E	Groundwater	926F/1392R	1,2,4-Trichlorobenzene & Dichlorobenzenes	3.28	Qiao et al., 2018 (66)
18	37.11 N 79.27 W	Wastewater	515F/806 R	PCBs	0.10	Mattes et al., 2018 (5)
19	45.75 N 126.63 E	Sludge	27F/533R	TCE	2.62	Chen et al., 2019 (67)
20	15.77 N 78.06 E	Sludge	515F/806 R	HCHs, DDTs	30	Raju et al., 2017 (68)
21	41.66 N 91.55 W	Groundwater	515F/806 R	VC	0.02	Liu et al., 2018 (69)
22	33.42 N 11.93 W	Groundwater	515F/806 R	TCE	464.80	Delgado et al., 2017 (70)

23	42.20 N 71.42 W	Groundwater	8F/1541R	PCE	2.49	Yang et al., 2015 (71)
24	15.77 N 78.06 E	Sediment	515F/806R	DDTs	5.00	Saghee et al., 2018 (72)
25	32.06 N 118.81 E	Soil	338F/806R	Hexachlorobenzene	3.80	Song et al., 2016 (73)
26	39.09 N 117.06 E	Soil	515F/806R	Herbicide metolachlor	10, 20	Li et al., 2018 (74)
27	47.51 N 10.09 E	Soil	27F/1492R	PCBs	0.0008	Weiland-Brauer et al., 2017 (6)
28	30.1 N 108.5 E	Soil	519F/907R	PCBs	60	Huang et al., 2018 (75)
29	50.74 N 3.11 E	Soil	341F/806R	Diverse pesticides	0.03	Holmsgaard et al., 2017 (76)
30	23.3 N 116.32 E	Sediment	515F/806R	PCBs	PCBs 6-164	Liu et al., 2018 (77)
31	23.93 N 113.48 E 23.55 N 113.67 E 23.32 N 116.33 E 28.53 N 121.38 E	Soil	341F/802R	PCBs	30-8780	Jiang et al., 2017 (78)

	28.53 N 121.42 E 24.92 N 67.50 E 30.23 N 71.48 E 31.53 N 74.33 E					
32	41.55 N 2.18 W	Wastewater	341F/907R	Dichloromethane	83	Trueba-Santiso et al., 2017 (79)
33	23.42 N 116.38 E	Soil	515F/806R	PCBs	0.73	Liu et al., 2015 (80)

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2.3 Microbial data analysis

2.3.1 Sequence raw data analysis

Referencing from Rognes (81) and Edgar (82), the raw data was analyzed by Vsearch with the major restrict conditions: 0.01 % filter rate, sizeout minuniquesize 2, and cluster 0.97% similarity. Taxonomy was assigned using the RDP database (83). The specific commands were listed below:

```
# 1) Set files
# .\db # database, copy rdp_16s_v16.fa and rdp_gold.fa beforehand
# .\seq # raw data
# .\temp # temp directory for intermediate files
# .\result # final results
# 2) Merge paired reads and label samples
vsearch --fastq_mergepairs .\seq\[forward fq file name] --reverse .\seq\[backward fq file name] --fastqout .\temp\[forward fq file name].merged.fq --relabel [forward fq file name].
# 3) Merge all files to a file via Python3.0
python.exe .\merge_file.py .\seq\
# 4) Cut primers and quality filter
vsearch --fastx_filter .\temp\all.fq --fastq_stripleft 18bp --fastq_stripright 18bp --fastqout .\temp\stripped.fq
# 5) fastq filter
vsearch --fastx_filter .\temp\stripped.fq --fastq_maxee_rate 0.01 --fastaout .\temp\filtered.fa
# 6) OTUs Dereplication and cluster otus
vsearch --derep_fulllength .\temp\filtered.fa --sizeout --minuniquesize 2 --output .\temp\uniques.fa
# 7) get OTUs table
vsearch --cluster_fast .\temp\uniques.fa --id 0.97 --centroids .\temp\otus.fa --relabel OTU_
# 8) remove chimeras
vsearch --uchime3_denovo .\temp\otus.fa --nonchimeras .\result\otus.fa
# 9) Create OTUs table
vsearch --usearch_global .\temp\filtered.fa --db .\result\otus.fa --id 0.97 --otutabout .\result\otutab.txt --threads 4
# 10) Species annotation
vsearch --sintax .\result\otus.fa --db .\db\rdp_16s_v16.fa --tabbedout .\result\out_tax.txt --strand both --sintax_cutoff 0.8 --threads 4
```

2.3.2 Microbial diversity analysis

After alignment, the OTUs were used to analyze microbial diversity (Shannon and Simpson) using the “vegan” (84) package of R software, then the results from each study were combined. Additionally, only methanogenic or OHRB OTUs were screened to calculate their Shannon or Simpson diversity indexes.

The specific commands were:

```
library("vegan")
data <- read.table ("clipboard",header = T,sep = '\t')
data_t <- t (data)
shannon<-diversity(data_t,index='shannon')
simpson<-diversity(data_t,index='simpson')
div<-data.frame(shannon,simpson)
write.csv(div,file= "div.csv", row.names = F,quote = F)
```

2.3.3 Meta-analysis

We classified the samples with OHRB or methanogen OTUs > 0 as '1' and the other samples as '0', to represent the presence and absence of OHRB or methanogens, respectively. Then, the random-effect model of the 'metafor' R package (85) was applied to analyze the effects of OHRB or methanogens on the Shannon or Simpson diversity indexes of total microbes. The specific commands were:

```
library(metafor)
mydata <- read.table ("clipboard",header = T,sep = '\t')
metamod<-rma(yi=Mean,data=mydata,sei=SEM,method="DL")
summary(metamod)
forestplot<-forest(metamod,refline = 1,mlab="Random-effect Model for All Studies",slab=paste(mydata$Type,mydata$N,sep=","),xlab="β",showweights = T)
```

2.3.4 Network analysis

The co-occurrence network was inferred based on the Spearman correlation matrix constructed using the 'psych' and 'WGCNA' packages of R software (86). We adjusted all *P*-values > 0.01, and the cutoff for direct correlation coefficients was determined as 0.7 through random matrix theory-based methods. Network topological characteristics were counted using 'Network analyzer' in Cytoscape 3.7.1 (87). The specific commands were:

```
library(WGCNA)
library(psych)
library(igraph)
#library(reshape2)
allowWGCNAThreads()
options(stringsAsFactors = FALSE)

exprMat = 'COMPLEX-ck'
```

```
data <- read.table ("clipboard",header = T,sep = '\t')
if (length(data)) {
   print("Start correlation analysis.")
   begin_time = Sys.time()
   occor = corr.test(data,use="pairwise",method="spearman",adjust="fdr",alpha=0.001)
   end_time = Sys.time()
   print("End correlation analysis.")
   paste("Time consuming: ", as.character.POSIXt(end_time - begin_time))
}
occor.r = occor$r
occor.p = occor$p
occor.r[occor.p>0.05|abs(occor.r)<0.7] = 0
write.csv(occor.r, paste(exprMat,"csv",sep="."))

TOM <- occor.r

if (dim(TOM)[1] != dim(TOM)[2])
for (i in c(1:dim(TOM)[1])) {
   for (j in c(1:dim(TOM)[2])) {
      if (is.na(TOM[i,j]) || is.na(TOM[j,i])) {
         TOM[i,j] = TOM[j,i] = NA
         next
      }
      if (TOM[i,j] != TOM[j,i]) {
         if (abs(TOM[i,j]) < abs(TOM[j,i])) {
            TOM[i,j] = TOM[j,i]
         }else{
            TOM[j,i] = TOM[i,j]
         }
      }
   }
}
'
i = 0
while (i <= dim(TOM)[1]) {
   i = i + 1
   if (i > dim(TOM)[1]) {
      next
   }
```

```
    if (sum(is.na(TOM[i,])) >= length(TOM[i,]) / 2) {
        TOM = TOM[-i,]
        TOM = TOM[,-i]
        i = i - 1
    }
}
'
# Export the network into edge and node list files that Cytoscape can read
cyt = exportNetworkToCytoscape(TOM,
                                edgeFile = paste(exprMat, ".edges.txt", sep=""),
                                nodeFile = paste(exprMat, ".nodes.txt", sep=""),
                                weighted = TRUE, threshold = -1)
```

2.4 Anaerobic incubation experiment

2.4.1 Medium of *M.* barkeri

Methanol..... 10.0 ml (Used in preculture and later replaced by acetate in formal incubation)

Acetate..... 10.0 ml (applied in formal incubation with γ-HCH)

K_2HPO_4 ..... 348.0 mg

KH_2PO_4 ..... 227.0 mg

NH_4Cl ..... 500.0 mg

$MgSO_4.7H_2O$ ..... 500.0 mg

$CaCl_2.2H_2O$ ..... 250.0 mg

$FeSO_4.7H_2O$ ..... 2.0 mg

Trace Elements Solution SL-6 (see below) .....3.0 ml

Wolfe's Vitamin Solution (see below) .....10.0 ml

Yeast Extract (BD 212750) .....2.0 g

Casitone (BD 225930) ..... 2.0 g

NaCl..... 2.25 g

Resazurin (0.025% solution) .....4.0 ml

NaHCO3 Solution (see below) ..... 20.0 ml

Reducing Agent (see below) ..... 20.0 ml

Agar..... 20.0 g

Distilled water..... 950.0 ml

Mix all of the ingredients except the Wolfe's Vitamin Solution, $NaHCO_3$ Solution, Methanol and Cysteine/Na_2S Solution (Reducing Agent) and autoclave for 15 minutes. After autoclaving, cool under 80% N_2, 20% CO_2 and add the solutions in the order listed above. Adjust pH to 6.8 if necessary and tube anaerobically and aseptically.

Trace Elements Solution SL-6:

$ZnSO_4.7H_2O$ .....0.10 g

$MnCl_2.4H_2O$ .....0.03 g

H_3BO_3 .....0.3 g

$CoCl_2.6H_2O$ .....0.2 g

$CuCl_2.2H_2O$ .....0.01 g

$NiCl_2.6H_2O$ .....0.02 g

$Na_2MoO_4.2H_2O$.....0.03 g

Distilled water.....1.0 L

Wolfe's Vitamin Solution:

Available from ATCC as a sterile ready-to-use liquid (Vitamin Supplement, catalog no. MD-VS).

Biotin.....2.0 mg

Folic acid.....2.0 mg

Pyridoxine hydrochloride.....10.0 mg

Thiamine. HCl.....5.0 mg

Riboflavin.....5.0 mg

Nicotinic acid.....5.0 mg

Calcium D-(+)-pantothenate.....5.0 mg

Vitamin B12.....0.1 mg

p-Aminobenzoic acid.....5.0 mg

Thioctic acid.....5.0 mg

Distilled water.....1.0 L

$NaHCO_3$ Solution:

Dissolve 850 mg of $NaHCO_3$ in 20.0 ml of water. After filter-sterilizing, equilibrate under CO_2 for 20 minutes.

Reducing Agent:

Add 300 mg L-cysteine. HCl to 10 ml of water and 300 mg $Na_2S.9H_2O$ to a second 10 ml of water; tube under nitrogen gas. After autoclaving at 121°C for 15 minutes under fast exhaust and allowing to cool, mix equal amounts of the cysteine and the sodium sulfide (under nitrogen). The mixture should be clear and can be used up to two weeks.

2.4.2 Untargeted metabolomic analysis

All samples were acquired by the LC-MS/MS system followed machine orders. The analytical conditions were as follows, UPLC: column, Waters ACQUITY UPLC HSS T3 C18 (1.8 μm, 2.1 mm*100 mm); column temperature, 35 ∘C; flow rate, 0.3 mL/min; injection volume, 1μL; solvent system, water (0.01% methanolic acid): acetonitrile; gradient program of positive ion, 95:5 V/V at 0 min, 79:21 V/V at 3.0 min, 50:50 V/V at 5.0 min, 30:70 V/V at 9.0 min, 5:95 V/V at 10.0 min , 95:5 V/V at 14.0 min; gradient program of negative ion, 95:5 V/V at 0 min, 79:21 V/V at 3.0 min, 50:50 V/V at 5.0 min, 30:70 V/V at 9.0 min, 5:95 V/V at 10.0 min , 95:5 V/V at 14.0 min.

The original data file obtained by LC-MS/MS analysis was firstly converted into mzML format by ProteoWizard software. Peak extraction, alignment and retention time correction were performed by XCMS program. The “SVR” method was used to correct the peak area, with the peaks filtered with deletion rate of > 50% in each group of samples. The differential metabolites were identified based on Human Metabolome (HMDB) or American Chemical Society (CAS) or Metlin database. Volcano Plots, column charts, and heatmaps were constructed via R program 4.0.1, to visualize the differences in metabolite levels for each comparison.

3 Results

3.1 Microbial diversity, Methanogen and OHRB

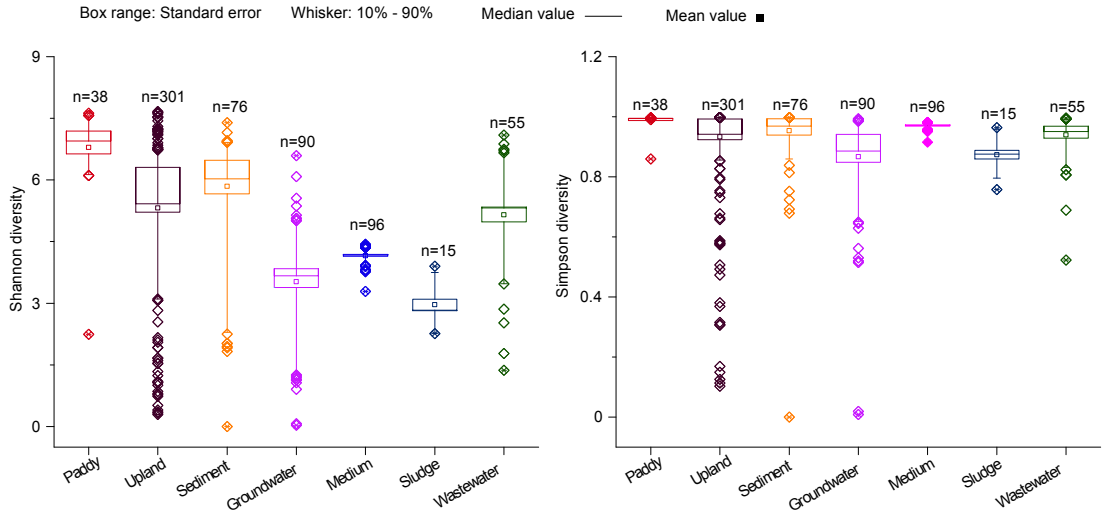

Fig. S1. Microbial Shannon and Simpson diversity

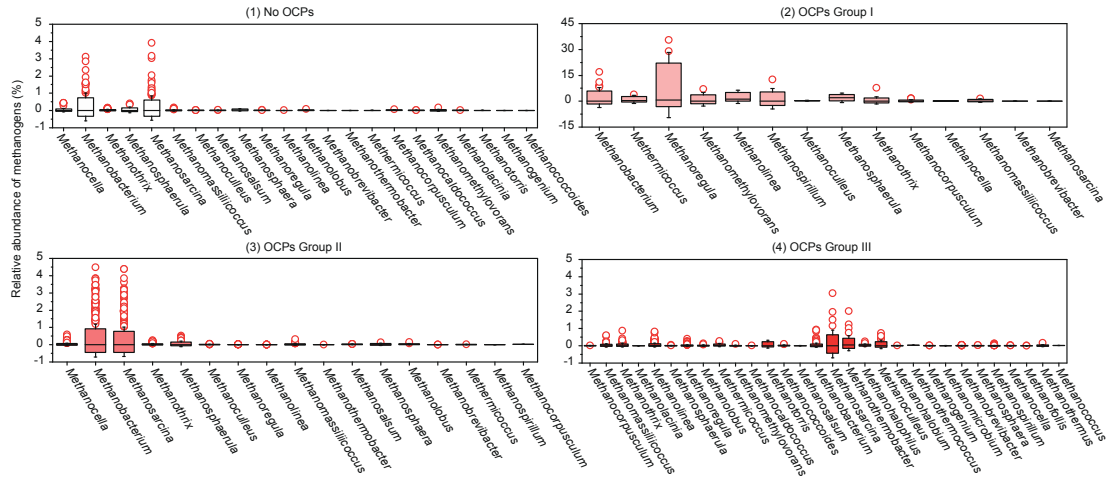

Fig. S2. The relative abundance of methanogens

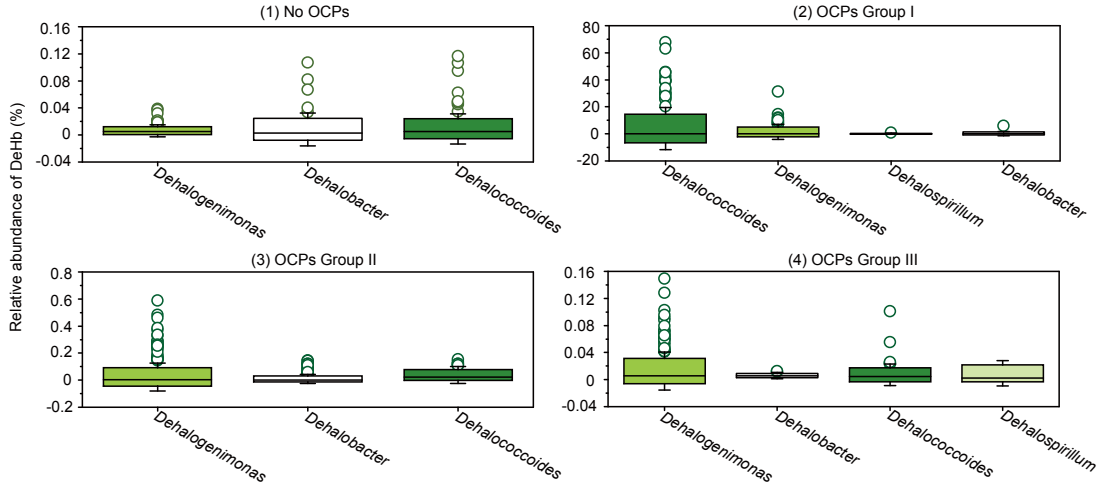

Fig. S3. The relative abundance of obligate dehalorespiration bacteria (OHRB)

3.2 List of dechlorinators

1) Obligate dehalorespiration bacteria (OHRB): *Dehalobacter*, *Dehalococcoides*, *Dehalogenimonas* and *Dehalospirillum.*

2) Co-metabolic dechlorination bacteria (CORB): With the exception of OHRB, other dechlorinators at genus level were included:

Achromobacter Acinetobacter Aeromonas Anaeromyxobacter Arthrobacter Bacillus Bosea Brevibacterium Burkholderia Caulobacter Chromobacterium Citrobacter Clostridium Comamonas Corynebacterium Cupriavidus Desulfitobacterium Desulfobacter Desulfococcus Desulfomonile Desulfovibrio Desulfuromonas Enterobacter Flavobacterium Geobacter Klebsiella Lactobacillus Methermicoccus Mycobacterium Nocardioides Novosphingobium Pseudomonas Pseudonocardia Pseudoxanthomonas Ralstonia Rhodococcus Saccharomonospora Sedimentibacter Serratia Shewanella Sphaerotilus Sphingobium Sphingomonas Staphylococcus Stenotrophomonas Streptomyces Sulfurospirillum Xanthomonas Zoogloea

At class level: *Actinobacteria*, *Alphaproteobacteria*, *Bacilli*, *Betaproteobacteria*, *Caldilineae*, *Clostridia*, *Deltaproteobacteria*, *Flavobacteriia*, *Gammaproteobacteria*

Table S4. Isolated dechlorinators

OCPs	Species	Genus	Class	Superkingdom
Atrazine (88-93)	*Klebsiella pneumonia*	*Klebsiella*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Rhodococcus corallines	*Rhodococcus*	*Actinobacteria*	Bacteria
	Myriophyllum spicatum	*Myriophyllum*	*Dicotyledons*	Bacteria
	Arthrobacter sp. C3	*Arthrobacter*	*Actinobacteria*	Bacteria
	Pseudomonas sp. ADP	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Rhizobium sp.	*Rhizobium*	*Alphaproteobacteria*	Bacteria
Aldrin (94-96)	*Anabaena sp. ARM 310*	*Anabaena*	*Synechococcophycideae*	Bacteria
	Aulosira fertilissima ARM 68	*Aulosira*	*Cyanophyceae*	Bacteria
	Pseudonocardia sp. KSF27	*Pseudonocardia*	*Actinobacteria*	Bacteria
	Arthrobacter sp	*Arthrobacter*	*Actinobacteria*	Bacteria
	Bacillus sp	*Bacillus*	*Bacilli*	Bacteria
	Burkholderia sp	*Burkholderia*	*Betaproteobacteria*	Bacteria
	Cupriavidus sp	*Cupriavidus*	*Betaproteobacteria*	Bacteria
	Micrococcus sp	*Micrococcus*	*Actinobacteria*	Bacteria

	Pseudomonas sp	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
Chlordane (97)	*Achromobacter delicatulus*	*Achromobacter*	*Betaproteobacteria*	Bacteria
	Bacillus megateriurn	*Bacillus*	*Bacilli*	Bacteria
	Bacillus subtilis	*Bacillus*	*Bacilli*	Bacteria
	Caulobacter vibrioides	*Caulobacter*	*Alphaproteobacteria*	Bacteria
	Chromobacterium violaceurn	*Chromobacterium*	*Betaproteobacteria*	Bacteria
	Enterobacter aerogenes	*Enterobacter*	*Gammaproteobacteria*	Bacteria
	Escherichia coli	*Escherichia*	*Gammaproteobacteria*	Bacteria
	Micrococcus roseus	*Micrococcus*	*Actinobacteria*	Bacteria
	Pseudomonas aeruginosa	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas fluorescens	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas putida	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Sphaerotilus natans	*Sphaerotilus*	*Betaproteobacteria*	Bacteria
	Zoogloea ramigera.	*Zoogloea*	*Betaproteobacteria*	Bacteria
Endosulfan (98-102)	*Acidovorax sp. KKS102*	*Acidovorax*	*Betaproteobacteria*	Bacteria
	Pseudomonas aeruginosa	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Mycobacterium sp.	*Mycobacterium*	*Actinobacteria*	Bacteria
	Arthrobacter sp.	*Arthrobacter*	*Actinobacteria*	Bacteria
	Enterobacter asburiae JAS5	*Enterobacter*	*Gammaproteobacteria*	Bacteria
	Enterobacter cloacae JAS7	*Enterobacter*	*Gammaproteobacteria*	Bacteria
Monochlorobenzene (103)	*Dehalobacter sp. TeCB1*	*Dehalobacter*	*Clostridia*	Bacteria
Dichlorobenzene (104, 105)	*Desulfomonile tiedjei*	*Desulfomonile*	*Deltaproteobacteria*	Bacteria
	Pseudomonas sp.	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
Tetrachlorobenzene (106, 107)	*Dehalobacter sp. TeCB1*	*Dehalobacter*	*Clostridia*	Bacteria
	Burkholderia PS12	*Burkholderia*	*Betaproteobacteria*	Bacteria
Dichlorodiphenyltrichloroethane (DDT) (108-111)	*Stenotrophomonas sp. DDT-1*	*Stenotrophomonas*	*Gammaproteobacteria*	Bacteria
	Aeromonas hydrophila HS01	*Aeromonas*	*Gammaproteobacteria*	Bacteria

	Pseudomonas sp.	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Klebsiella pneumonia	*Klebsiella*	*Gammaproteobacteria*	Bacteria
	Agrobacterium	*Agrobacterium*	*Alphaproteobacteria*	Bacteria
	Alcaligenes	*Alcaligenes*	*Betaproteobacteria*	Bacteria
	Clostridium	*Clostridium*	*Clostridia*	Bacteria
	Dehalospirillum multivorans	*Dehalospirillum*	*Epsilonproteobacteria*	Bacteria
	Hydrogenomonas	*Hydrogenomonas*	*Epsilonproteobacteria*	Bacteria
	Pseudoxanthomonas jiangsuensis	*Pseudoxanthomonas*	*Gammaproteobacteria*	Bacteria
	Staphylococcus	*Staphylococcus*	*Bacilli*	Bacteria
	Stenotrophomonas	*Stenotrophomonas*	*Gammaproteobacteria*	Bacteria
	Streptomyces	*Streptomyces*	*Actinobacteria*	Bacteria
	Xanthomonas	*Xanthomonas*	*Gammaproteobacteria*	Bacteria
	Xerocumus chrysenteron	*Xerocumus*	*Agaricomycotina*	Fungi
Dieldrin Endrin (112, 113)	*Pseudomonas fluorescens*	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.27	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.33	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.34	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.103	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.105	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.117	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.138	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Pseudomonas sp.265	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Micrococcus sp.204	*Micrococcus*	*Actinobacteria*	Bacteria
	Bacillus sp.458	*Bacillus*	*Bacilli*	Bacteria
	Bacillus sp.459	*Bacillus*	*Bacilli*	Bacteria
	Bacillus sp.461	*Bacillus*	*Bacilli*	Bacteria

	Arthrobacter sp.278	*Arthrobacter*	*Actinobacteria*	Bacteria
	Burkholderia sp.	*Burkholderia*	*Betaproteobacteria*	Bacteria
	Cupriavidus sp.	*Cupriavidus*	*Betaproteobacteria*	Bacteria
	Burkholderia sp.	*Burkholderia*	*Betaproteobacteria*	Bacteria
	Mucor racemosus	*Mucor*	*Mucoromycotina*	Fungi
Heptachlor (114)	*Phlebia tremellosa*	*Phlebia*	*Agaricomycotina*	Fungi
	Phlebia brevispora,	*Phlebia*	*Agaricomycotina*	Fungi
	Phlebia acanthocystis	*Phlebia*	*Agaricomycotina*	Fungi
Hexachlorocyclohexane (HCH) (115-126)	*Sphingobium spp.*	*Sphingobium*	*Alphaproteobacteria*	Bacteria
	Bacillus sp.	*Bacillus*	*Bacilli*	Bacteria
	Xanthomonas sp. ICH12	*Xanthomonas*	*Gammaproteobacteria*	Bacteria
	Sphingomonas quisquiliarum	*Sphingomonas*	*Alphaproteobacteria*	Bacteria
	Clostridium sphenoides	*Clostridium*	*Clostridia*	Bacteria
	Serratia marcescens	*Serratia*	*Gammaproteobacteria*	Bacteria
	Proteus mirabilis	*Proteus*	*Gammaproteobacteria*	Bacteria
	P. Vulgaris	*Proteus*	*Gammaproteobacteria*	Bacteria
	Clostridium rectum	*Clostridium*	*Clostridia*	Bacteria
	Clostridia	*Clostridium*	*Clostridia*	Bacteria
	Clostridium rectumstrain S-17	*Clostridium*	*Clostridia*	Bacteria
	C. bifermentans	*Clostridium*	*Clostridia*	Bacteria
	C. sporogenes	*Clostridium*	*Clostridia*	Bacteria
	C. putrefaciens	*Clostridium*	*Clostridia*	Bacteria
	C. lentoputrescens	*Clostridium*	*Clostridia*	Bacteria
	C. butyricum	*Clostridium*	*Clostridia*	Bacteria
	C. acetobutylicum	*Clostridium*	*Clostridia*	Bacteria
	C. histolyticum	*Clostridium*	*Clostridia*	Bacteria
	Dehalobacter	*Dehalobacter*	*Clostridia*	Bacteria
	Sedimentibacter sp.	*Sedimentibacter*	*Clostridia*	Bacteria
	Dehalobacter sp. E1	*Dehalobacter*	*Clostridia*	Bacteria
	Desulfococcus multivorans DSM2059	*Desulfococcus*	*Deltaproteobacteria*	Bacteria
	Desulfovibrio gigas DSM 1382	*Desulfovibrio*	*Deltaproteobacteria*	Bacteria
	Clostridium bifermentans	*Clostridium*	*Clostridia*	Bacteria
	Clostridium glycolium	*Clostridium*	*Clostridia*	Bacteria
	Clostridium sp.	*Clostridium*	*Clostridia*	Bacteria

	Desulfovibrio gigas ATCC 19364	*Desulfovibrio*	*Deltaproteobacteria*	Bacteria
	Desulfovibrio africanus ATCC 19997	*Desulfovibrio*	*Deltaproteobacteria*	Bacteria
	Desulfobacter curvatus ATCC 43919	*Desulfobacter*	*Deltaproteobacteria*	Bacteria
	Desulfococcus multivorans ATCC 33890	*Desulfococcus*	*Deltaproteobacteria*	Bacteria
	Bosea thiooxidans	*Bosea*	*Alphaproteobacteria*	Bacteria
	Pseudomonas paucimobilis	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Sphingomonas paucimobilis UT26	*Sphingomonas*	*Alphaproteobacteria*	Bacteria
	Trametes hirsutus	*Trametes*	*Agaricomycotina*	Fungi
Methoxychlor (127, 128)	*Enterobacter aerogenes*	*Enterobacter*	*Gammaproteobacteria*	Bacteria
	Bradyrhizobium sp. 17-4	*Bradyrhizobium*	*Alphaproteobacteria*	Bacteria
Mirex (129)	*Bacillus sphaericus*	*Bacillus*	*Bacilli*	Bacteria
	Streptomyces albus	*Streptomyces*	*Actinobacteria*	Bacteria
Poly-o-chlorinated dibenzodioxin (PCDDs) (130, 131)	*Dehalococcoides mccartyi 195*	*Dehalococcoides*	*Dehalococcoidia*	Bacteria
	Dehalobacter sp.	*Dehalobacter*	*Clostridia*	Bacteria
Pentachlorophenol (PCP) Trichlorophenol (TCP) Dichlorophenol (DCP) (132-168)	*Abortiporus biemmis HR145*	*Abortiporus*	*Agaricomycotina*	Fungi
	Oudemansiella australis HR345	*Oudemansiella*	*Agaricomycotina*	Fungi
	Stereum fasciatum HR348	*Stereum*	*Agaricomycotina*	Fungi
	Rigidoporus catervatus HR316	*Rigidoporus*	*Agaricomycotina*	Fungi
	Absidia fusca	*Absidia*	*Mucoromycotina*	Fungi
	Acinetobacter sp. ISTPCP-3	*Acinetobacter*	*Gammaproteobacteria*	Bacteria
	Agrobacterium radiobacter	*Agrobacterium*	*Alphaproteobacteria*	Bacteria
	Agrocybe perfecta CCB161	*Agrocybe*	*Agaricomycotina*	Fungi
	Peniophora cinerea CCB204	*Peniophora*	*Agaricomycotina*	Fungi
	Psilocybe castanella CCB444	*Psilocybe*	*Agaricomycotina*	Fungi
	Amylomyces rouxii	*Amylomyces*	*Mucoromycotina*	Fungi
	Anthracophyllum discolor	*Anthracophyllum*	*Agaricomycotina*	Fungi
	Armillaria gallica 1039	*Armillaria*	*Agaricomycotina*	Fungi
	Ganoderma lucidum HK-1	*Ganoderma*	*Agaricomycotina*	Fungi
	Polyporus sp. Cv-1	*Polyporus*	*Agaricomycotina*	Fungi
	Volvariella volvacea V34	*Volvariella*	*Agaricomycotina*	Fungi

	Arthrobacter sp. ATCC 33790	*Arthrobacter*	*Actinobacteria*	Bacteria
	Bacillus sp.	*Bacillus*	*Bacilli*	Bacteria
	Staphylococcus sp.	*Staphylococcus*	*Bacilli*	Bacteria
	Bjerkandera adusta ATTC 90940	*Bjerkandera*	*Agaricomycotina*	Fungi
	Brevibacterium casei TVS-3	*Brevibacterium*	*Actinobacteria*	Bacteria
	Byssochlamys fulva	*Byssochlamys*	*Pezizomycotina*	Fungi
	Candidatus comitans K112	*Sphingobacterium*	*Sphingobacteriia*	Bacteria
	Mucor ramonissimus IM 6203	*Mucor*	*Mucoromycotina*	Fungi
	Paraconiothyrium variabile	*Paraconiothyrium*	*Pezizomycotina*	Fungi
	Sphingomonas sp. K6	*Sphingomonas*	*Alphaproteobacteria*	Bacteria
	Nocardioides sp. K103	*Nocardioides*	*Actinobacteria*	Bacteria
	Chrysonilia sitophila DSM 16514	*Chrysonilia*	*Pezizomycotina*	Fungi
	Penicillium hirayamae	*Penicillium*	*Pezizomycotina*	Fungi
	Trichoderma longibrachiatum DSM 16517	*Trichoderma*	*Pezizomycotina*	Fungi
	Cladosporium herbarum	*Cladosporium*	*Pezizomycotina*	Fungi
	Coriolus versicolor	*Coriolus*	*Agaricomycotina*	Fungi
	Desulfitobacterium hafniense PCP-1	*Desulfitobacterium*	*Clostridia*	Bacteria
	Escherichia coli	*Escherichia*	*Gammaproteobacteria*	Bacteria
	Flavobacterium sp. ATCC53874	*Flavobacterium*	*Flavobacteriia*	Bacteria
	Fomes fomentarius	*Fomes*	*Agaricomycotina*	Fungi
	Laetiporus Cincinnatus	*Laetiporus*	*Agaricomycotina*	Fungi
	Galerina patagônica Sp3	*Galerina*	*Agaricomycotina*	Fungi
	Inonotus sp. Sp2	*Inonotus*	*Agaricomycotina*	Fungi
	Lenzites betulina Ru-30	*Lenzites*	*Agaricomycotina*	Fungi
	Gloeophyllum striatum DSM 9592	*Gloeophyllum*	*Agaricomycotina*	Fungi
	Irpex lacteus ATCC 11245	*Irpex*	*Agaricomycotina*	Fungi
	Kocuria sp. CL2	*Kocuria*	*Actinobacteria*	Bacteria
	Lentinula edodes LE2	*Lentinula*	*Agaricomycotina*	Fungi
	Mycobacterium chlorophenolicum	*Mycobacterium*	*Actinobacteria*	Bacteria
	Novosphingobium sp. MT1	*Novosphingobium*	*Alphaproteobacteria*	Bacteria
	Penicillium camemberti	*Penicillium*	*Pezizomycotina*	Fungi
	Phanerochaete chrysosporium BMK-F-1767	*Phanerochaete*	*Agaricomycotina*	Fungi
	Pleurotus pulmonarius	*Pleurotus*	*Agaricomycotina*	Fungi
	Pseudomonas testosteroni CCM 7350	*Pseudomonas*	*Gammaproteobacteria*	Bacteria

	Rhizopus nigricans	*Rhizopus*	*Mucoromycotina*	Fungi
	Saccharomonospora viridis	*Saccharomonospora*	*Actinobacteria*	Bacteria
	Serratia marcescens AY927692	*Serratia*	*Gammaproteobacteria*	Bacteria
	Sphingobium chlorophenolicum	*Sphingobium*	*Alphaproteobacteria*	Bacteria
	Trametes pubescens	*Trametes*	*Agaricomycotina*	Fungi
Polychlorinated biphenyl (PCB) (169-181)	*Alcaligenes eutrophus H850*	*Alcaligenes*	*Betaproteobacteria*	Bacteria
	Alcaligenes faecalis	*Alcaligenes*	*Betaproteobacteria*	Bacteria
	Achromobacter sp. NP03	*Achromobacter*	*Betaproteobacteria*	Bacteria
	Acinetobacter caloaceticus	*Acinetobacter*	*Gammaproteobacteria*	Bacteria
	Comamonas acidovorans	*Comamonas*	*Betaproteobacteria*	Bacteria
	Flavobacterium devorans	*Flavobacterium*	*Flavobacteriia*	Bacteria
	Bacillus lentus	*Bacillus*	*Bacilli*	Bacteria
	Bacillus mascerans	*Bacillus*	*Bacilli*	Bacteria
	Bacillus thuringiensis	*Bacillus*	*Bacilli*	Bacteria
	Burkholderia sp. SRS-W-2-2016	*Burkholderia*	*Betaproteobacteria*	Bacteria
	Corynebacterium sp.	*Corynebacterium*	*Actinobacteria*	Bacteria
	Dehalococcoides mccartyi JNA	*Dehalococcoides*	*Dehalococcoidia*	Bacteria
	Pleurotus ostreatus	*Pleurotus*	*Agaricomycotina*	Fungi
	Nocardioides aromaticivorans IC177	*Nocardioides*	*Actinobacteria*	Bacteria
	Pseudomonas fluorescens F113	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Sphingomonas sp. N-9	*Sphingomonas*	*Alphaproteobacteria*	Bacteria
	Ralstonia eutropha H850	*Ralstonia*	*Betaproteobacteria*	Bacteria
	Rhodococcus sp. RHA1	*Rhodococcus*	*Actinobacteria*	Bacteria
Pentachloronitrobenzene (182)	*Cupriavidus sp. YNS-85*	*Cupriavidus*	*Betaproteobacteria*	Bacteria
Tetrachloroethylene Trichloroethylene Dichloroethylene Vinyl Chloride (183-189)	*Dehalobacter sp.*	*Dehalobacter*	*Clostridia*	Bacteria
	Clostridium bifermentans DPH-1	*Clostridium*	*Clostridia*	Bacteria
	Desulfitobacterium hafniense JH1	*Desulfitobacterium*	*Clostridia*	Bacteria
	Desulfuromonas michiganensis sp. nov.	*Desulfuromonas*	*Deltaproteobacteria*	Bacteria
	Dehalococcoides sp. MB	*Dehalococcoides*	*Dehalococcoidia*	Bacteria

	Sulfurospirillum multivorans	*Sulfurospirillum*	*Epsilonproteobacteria*	Bacteria
	Desulfitobacterium sp. PCE-S	*Desulfitobacterium*	*Clostridia*	Bacteria
	Geobacter lovleyi sp. nov. SZ	*Geobacter*	*Deltaproteobacteria*	Bacteria
	Dehalococcoides mccartyi	*Dehalococcoides*	*Dehalococcoidia*	Bacteria
Toxaphene (190-192)	*Enterobacter cloacae D1*	*Enterobacter*	*Gammaproteobacteria*	Bacteria
	Pseudomonas putida	*Pseudomonas*	*Gammaproteobacteria*	Bacteria
	Bjerkandera sp. BOL13	*Bjerkandera*	*Agaricomycotina*	Fungi
Pentachloroethane Tetrachloroethane Trichloroethane Dichloroethane (193-199)	*Shewanella oneidensis MR-1*	*Shewanella*	*Gammaproteobacteria*	Bacteria
	Dehalogenimonas sp. WBC-2	*Dehalogenimonas*	*Dehalococcoidetes*	Bacteria
	Desulfitobacterium sp strain Y51	*Desulfitobacterium*	*Clostridia*	Bacteria
	Dehalogenimonas alkenigignens sp nov.	*Dehalogenimonas*	*Dehalococcoidetes*	Bacteria
	Dehalobacter sp.	*Dehalobacter*	*Clostridia*	Bacteria
	Dehalobacter sp. UNSWDHB	*Dehalobacter*	*Clostridia*	Bacteria
	Desulfitobacterium sp strain PR	*Desulfitobacterium*	*Clostridia*	Bacteria
Trichlorophenol (200)	*Ralstonia eutropha JMP134*	*Ralstonia*	*Betaproteobacteria*	Bacteria
Chlorobenzene (201)	*Dehalococcoides sp. CBDB1*	*Dehalococcoides*	*Dehalococcoidia*	Bacteria

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3.2 Dechlorination products found in *M*. barkari intracellular and extracellular

Table S5 Dechlorination products found in *M*. barkari intracellular and extracellular

Mode	Dechlorination products	Intracellular		Extracellular	
		no pollu	pollu	no pollu	pollu
Negative	gamma-Pentachlorocyclohexene (C6H5Cl5)	1.00	124.67	1.00	122.00
	1,3,4,6-Tetrachloro-1,4-cyclohexadiene (C6H4Cl4)	12512.74	23271.41	8713.88	10087.39
	delta-3,4,5,6-Tetrachlorocyclohexene;3,4,5,6-Tetrachlorocyclohexene (C6H6Cl4)	5082.68	4131.33	8031.24	4649.48
	Benzene, 1,3-dichloro- (C6H4Cl2)	128.48	4137.36	396.38	987.10
	1,2,3,4-Tetrachlorobenzene (C6H2Cl4)	1592.00	13105.08	1290.13	4677.58
	5,6-Dichloro-1,3-cyclohexadiene (C6H6Cl2)	1.00	2418.45	814.14	2105.48
Positive	gamma-Pentachlorocyclohexene (C6H5Cl5)	187.30	498.74	106.36	384.05
	3,4,5,6-Tetrachlorocyclohexene (C6H6Cl4)	745.83	2377.76	1278.70	1758.93
	1,4-Dichlorobenzene (C6H4Cl2)	1502.07	2937.87	779.41	276.72
	1,2,4-Trichlorobenzene (C6H3Cl3)	424.60	2331.98	658.24	394.00
	5,6-Dichloro-1,3-cyclohexadiene (C6H6Cl2)	624.31	2325.43	817.21	1441.91
	1,2,3,4,5-Pentachlorobenzene (C6HCl5)	616.38	367.55	114.71	117.12
	Chlorobenzene (C6H5Cl)	1483.80	1556.51	1.00	1.00

Number is the average peak in LC-MS/MS for each treatment.

3.3 Differential metabolites selection of *M*. barkari intracellular

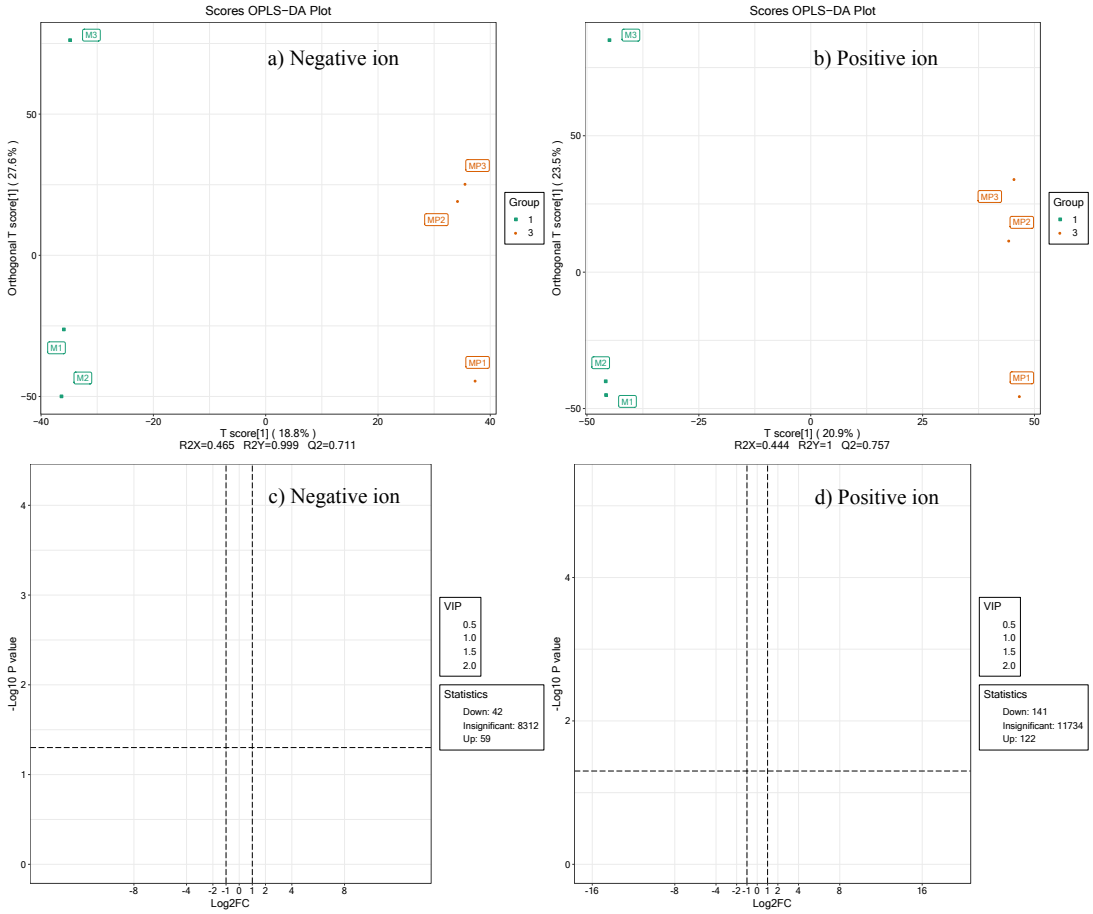

Fig. S4 OPLS_DA and volcano plots of differential metabolites selection of *M*. barkari intracellular

The comparison is between: with/without of γ-HCH.

282 **Table S6 Differential metabolites list of *M*. barkari intracellular between with/without γ-HCH**

Mode	Type	Intracellular
Negative	Up (37)	p-Salicylic acid (C7H6O3)
		PE-NMe2(18:2(9Z,12Z)/20:0) (C45H86NO8P)
		PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/24:0) (C52H90NO10P)
		Phe Lys Glu Ala Phe (C32H44N6O8)
		Clupanodonyl nitine (C27H54NO5)
		di-trans,poly-cis-Decaprenyl diphosphate;ditrans,heptacis-Decaprenyl diphosphate (C50H84O7P2)
		6-{[7,8,8,13,21,22-hexahydroxy-19-(hydroxymethyl)-3,6,16-trioxo-2,17,20,23-tetraoxapentacyclo[16.3.1.1,(1)(1).0,.0(1),(1)]tricosa-4,10,12,14-tetraen-12-yl]oxy}-3,4,5-trihydroxyoxane-2-carboxylic acid (C26H26O21)
		MLS001306483-01!Cytoxan6055-19-2 (C7H17Cl2N2O3P)
		5-Hydroxyindoleacetylglycine (C12H12N2O4)
		Fentin hydroxide; Fentin (C18H16OSn)
		PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/24:1(15Z)) (C52H88NO10P)
		Furosemide; LC-ESI-ITFT; MS2; CE (C12H11ClN2O5S)
		Flumetralin (C16H12ClF4N3O4)
		Cyclohexane-1,3-dione; 1,3-Cyclohexanedione; Dihydroresorcinol (C6H8O2)
		PysoPE 20:5 (C25H42NO7P)
		H-89 (C20H20BrN3O2S)
		1,3,7-Trimethyluric acid;1,3,7-Trimethylurate (C8H10N4O3)
		-Naphthylthiourea (C11H10N2S)
		DG(10:0/0:0/a-21:0) (C34H66O5)
		Lys Phe Ile (C21H34N4O4)
		Glutathionylspermine (C20H41N7O5S)
		PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:1(13Z)) (C50H84NO10P)
		MADECASSIC ACID (C30H48O6)
		C-12 NBD-dihydro-Ceramide (C36H63N5O6)
		Sulfate (H2O4S)
		Megalomicin C1 (C48H84N2O17)
		Carbenicillin (C17H18N2O6S)
		PA(20:3(5Z,8Z,11Z)/22:0) (C45H83O8P)
		Thalassemine; L-Thalassemine (C8H19N4O6P)
		Miconazole (C18H14Cl4N2O)
		His Arg Leu Leu Leu (C30H54N10O6)
		Cammaconine; Columbiananine (C23H37NO5)
		Modafinil acid (C15H14O3S)
		ROXITHROMYCIN (C41H76N2O15)

		Oleoyl 3-carbacyclic Phosphatidic Acid (C22H41O5P) Chloroacetaldehyde; 2-Chloroethanal (C2H3ClO) PE-NMe2(9D5/13M5) (C50H88NO10P)
	Down (25)	Purpureacin-1 (C37H66O8) Bougainvillein-r-I; Bougainvillein-v (C30H36N2O18) Thymophthalein (C28H30O4) MAM2201 N-(4-hydroxypentyl) metabolite (C25H24FNO2) UCL 1684; 6,10-Diaza-3(1,3)8,(1,4)-dibenzena-1,5(1,4)-diquinolinacyclodecaphane (C34H30N4) (S)-3-Sulfonatolactate (C3H6O6S) 1-(naphthalen-2-yl)-2-[(6-nitro-1,3-benzothiazol-2-yl)sulfanyl]ethenone (C19H12N2O3S2) Vitamin K1 epoxide; (2,3-Epoxyphytyl)menaquinone; 2,3-Epoxy-2,3-dihydro-2-methyl-3-phytyl-1,4-naphthoquinone; 2,3-Epoxyphylloquinone; 1a,7a-Dihydro-1a-methyl-7a-(3,7,11,15-tetramethyl-2-hexadecenyl)-naphth[2,3-b]oxirene-2,7-dione; Phylloquinone oxide; Phylloquinone epoxide; Phylloquinone-2,3-epoxide; Vitamin K1 2,3-epoxide; Vitamin K1 oxide (C31H46O3) PG(i-12:0/i-20:0) (C38H75O10P) PG(i-12:0/a-25:0) (C43H85O10P) N-(4,7-Dihydroxy-8-methyl-2-oxo-2H-chromen-3-yl)-2,2-dimethylchromane-6-carboxamide (C22H21NO6) Ergosta-5,7,22,24(28)-tetraen-3beta-ol; Ergosta-5,7,22,24(24(1))-tetraen-3beta-ol;5,7,22,24(28)-Ergostatetraenol (C28H42O) Pro Val Ala Glu Val (C23H39N5O8) PA(16:0/24:0) (C43H85O8P) HexCer-NS d34:2 (C40H75NO8) Ioxitalamic acid (C12H11I3N2O5) DG(9D3/13D5/0:0) (C45H76O7) PI(20:4(5Z,8Z,11Z,14Z)/16:0) (C45H79O13P) Octaethylene glycol (C16H34O9) Opipramol (C23H29N3O) Hexacosane (C26H54) 3,4,3',4'-Tetrahydrospirilloxanthin (C42H64O2) PC(18:2(9Z,12Z)/18:2(9Z,12Z)) (C44H80NO8P) PS(20:1(11Z)/24:0) (C50H96NO10P) beta-D-Mannosylphosphodecaprenol (C56H93O9P)
Positive	Up (84)	alpha-D-Ribose 1-methylphosphonate 5-triphosphate (C6H16O16P4) MG(18:0) (C21H43O4) Mertansine; DM 1 (C35H48ClN3O10S) Iloperidone (C24H27FN2O4) PA(20:4(5Z,8Z,11Z,14Z)/24:0) (C47H85O8P)

		Leu Gln Arg Arg (C23H45N11O6)
		Aspartylglycosamine (C12H21N3O8)
		Cycloastragenol (C30H50O5)
		Asp Ser Asn (C11H18N4O8)
		Triadimenol (C14H18ClN3O2)
		Diosmin (C28H32O15)
		Dihydrozein-O-glucoside (C16H25N5O6)
		1-Hexadecanol; Hexadecanol; Cetyl alcohol; Palmityl alcohol; 16-Hexadecanol (C16H34O)
		Portulacaxanthin III (C11H12N2O6)
		Trp-HoPhe-OH (C27H25N3O6)
		Aminomalonate; Aminomalonic acid; 2-Aminomalonic acid (C3H5NO4)
		Saxagliptin (C18H25N3O2)
		DG(22:1(13Z)/19:2(10Z,13Z)/0:0) (C44H80O5)
		Glycine deoxycholic acid (C26H43NO5.H2O)
		Arg Asp Leu Tyr Ser (C28H44N8O10)
		Lys Cys Ala (C12H24N4O4S1)
		PG(16:0/18:1(9Z))[U] (C40H77O10P)
		4-(3-Methylbut-2-enyl)-L-tryptophan; 4-Dimethylallyl-L-tryptophan (C16H20N2O2)
		Arg Val Ile Trp Gly (C30H47N9O6)
		Lovastatin (C24H36O5)
		3-(Phosphoacetylamido)-L-alanine (C5H11N2O7P)
		Phe Cys Thr (C16H23N3O5S1)
		5-O-Methylvisamminol (C16H18O5)
		Gymnodimine; Gymnodimine A; GYM A (C32H45NO4)
		Methylmethionine sulfonium salt; Methylmethionine sulfonium chloride; Vitamin U (C6H14NO2S.Cl)
		3,4-Dimethyl-5-pentyl-2-furandodecanoic acid (C23H40O3)
		alpha-Narcotine; Noscapine (C22H23NO7)
		17beta-(Benzoyloxy)-B-norandrost-4-en-3-one (C25H30O3)
		4-Hydroxymethylimidazole (C4H6N2O)
		TG(i-24:0/20:0/17:0) (C64H124O6)
		Salicin 6-phosphate; Salicin-6P (C13H19O10P)
		LL-2,6-Diaminoheptanedioate; LL-2,6-Diaminopimelate; LL-2,6-Diaminopimelic acid (C7H14N2O4)
		Oxaloacetate; Oxalacetic acid; Oxaloacetic acid; 2-Oxobutanedioic acid;2-Oxosuccinic acid;keto-Oxaloacetate (C4H4O5)
		Proparacaine; Proxymetacaine (C16H26N2O3)
		TG(21:0/18:0/8:0) (C50H96O6)
		9-Fluoro-11beta-hydroxy-16beta-methylandrosta-1,4-diene-3,17-dione (C20H25FO3)
		N-Oxyclozapine (C18H19ClN4O)

		His Asn Ile Asp (C20H31N7O8) sulfamethoxazole hydroxylamine (C10H11N3O4S) 5 -Androst-16-en-3-ol (C19H30O) Methylisopelletierine (C9H17NO) beta-Carotene; all-trans-beta-Carotene (C40H56) Arachidonoyl 2'-Chloroethylamide (C22H36ClNO) Val Gln Ala Arg (C19H36N8O6) L-Glutamyl 5-phosphate; L-Glutamate 5-phosphate (C5H10NO7P) Pipotiazine (C24H33N3O3S2) Compound III(S); 5-(7-(4-(4-Ethyl-4,5-dihydrooxazol-2-yl)phenoxy)heptyl)-3-methylisoxazole (C22H30N2O3) Myristoyl-L-carnitine (C21H41NO4) Cypridina luciferin (C22H27N7O) Cyanopeptolin A (C46H72N10O12) 17-Epiestriol (C18H24O3) 4-Hydroxyphenylethanol (C8H10O2) Gly Leu Asp Val Trp (C28H40N6O8) Fortimicin FU-10 (C12H24N2O9) Glucoerucin (C12H23NO9S3) Carboxin (C12H13NO2S) 1-Diphosinositol pentakisphosphate; D-myo-Inositol, 2,3,4,5,6-pentakis(dihydrogen phosphate) 1-(trihydrogen diphosphate); Diphospho-myo-inositol pentakisphosphate; 1D-myo-Inositol 1-diphosphate 2,3,4,5,6-pentakisphosphate (C6H19O27P7) CITCO; 6-(4-Chlorophenyl)imidazo[2,1-b][1,3]thiazole-5-carbaldehyde O-(3,4-dichlorobenzyl)oxime (C19H12Cl3N3OS) Ecdysone palmitate; Ecdysone 3-palmitate (C43H74O7) Histamine; 1H-Imidazole-4-ethanamine; 2-(4-Imidazolyl)ethylamine (C5H9N3) 2-C-Methyl-D-erythritol 2,4-cyclodiphosphate; 3-Methyl-1,2,3,4-tetrahydroxybutane-1,3-cyclic bisphosphate (C5H12O9P2) 1,26-Hexacosanediol diferulate (C46H70O8) CAY10578 (C10H3I4NO4) Fumaric acid (C4H4O4) dCDP; 2'-Deoxycytidine diphosphate; 2'-Deoxycytidine 5'-diphosphate (C9H15N3O10P2) 3,4-Dihydrospheroidene; Methoxyneurosporene (C41H62O) Dalcetrapib (C23H35NO2S) (-)-alpha-Narcotine (C22H23NO7) 14,16-Hentriacontanedione; Hentriacontane-14,16-dione (C31H60O2) Ametryn (C9H17N5S)

		PE-NMe2(9D3/9M5) (C44H76NO10P) Naptalam; N-1-Naphthylphthalamic acid (C18H13NO3) Benzo[a]pyrene-7,8-diol; Benzo[a]pyrene-7,8-dihydrodiol (C20H14O2) Cer-AP t43:0 (C43H87NO5) Decylubiquinol; 6-Decylubiquinol; 2-Decyl-5,6-dimethoxy-3-methyl-1,4-benzenediol (C19H32O4) Glu Asp Gln Asp (C18H27N5O12) Bacteriohopanetetrol; Tetrahydroxybacteriohopane; Bacteriohopane-32,33,34,35-tetrol (C35H62O4) 17Z-hexacosenoic acid (C26H50O2) EUK 134 (C18H18ClMnN2O4)
	Down (97)	beta-Rhodomycin; Rhodomycin B (C28H33NO10) CAY10449 (C19H21N3O2) 2,6-Di-tert-butyl-4-hydroxymethylphenol (C15H24O2) PC(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)) (C44H76NO8P) SILDENAFIL (C22H30N6O4S) Chloroacetic acid (C2H3ClO2) Acetamide (C2H5NO) DROFENINE (C20H31NO2) L-erythro MAPP (C23H39NO2) 13-chloro-5,14-dihydroxy-7,12-dimethyl-6-(3-methylbut-2-en-1-yl)-10-oxo-2,9-dioxatricyclo[9.4.0.0(3),]pentadeca-1(15),3(8),4,6,11,13-hexaene-15-carbaldehyde (C21H19ClO6) CL(i-14:0/i-14:0/a-17:0/18:2(9Z,11Z))[rac] (C72H136O17P2) NS-102 (C12H11N3O4) SULFADIMETHOXINE (C12H14N4O4S) Antibiotic JI-20B; JI-20B (C20H41N5O9) Phenyl 5-phospho-alpha-D-ribofuranoside (C11H15O8P) Valerianine (C11H15NO) Triphenylphosphine oxide (C18H15OP) 2-Amino-4-oxo-4-alpha-hydroxy-6-(erythro-1',2',3'-trihydroxypropyl)-5,6,7,8-tetrahydroxypterin (C9H15N5O8) Ser Thr Trp (C18H24N4O6) D-Glucosaminate-6-phosphate; 2-Amino-2-deoxy-D-gluconate 6-phosphate (C6H14NO9P) ApNA (C26H36N2O3) Val Ser Trp (C19H26N4O5) Lys Tyr Ala Asp (C22H33N5O8) KN-62 (C38H35N5O6S2) N-benzyl-1-methyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine (C13H13N5) PGP(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:4(5Z,8Z,11Z,14Z)) (C48H76O13P2) Iprovalicarb (C18H28N2O3)

		1-Palmitoyl-2-(5-keto-8-oxo-6-octenoyl)-sn-glycero-3-phosphatidylcholine (C32H58NO10P)
		2,3,4,7,8,9,15,22,23,28-decahydroxy-14-(hydroxymethyl)-13,25,32,35-tetraoxaoctacyclo[14.13.3.3(1),(2).0,(3).0,(1)(1).0(1),(2).0(1),(2).0(2),(3)(3)]pentatriaconta-1,3,5(30),6,8,10,19(24),20,22,28-decaene-12,27,31,34-tetrone (C32H22O19)
		Sulthiame (C10H14N2O4S2)
		Atrazine-desethyl-desisopropyl (C3H4ClN5)
		PE-NMe(14:1(9Z)/20:0) (C40H78NO8P)
		Ser Glu Lys Arg (C20H38N8O8)
		Putrescine (C4H12N2)
		TG(i-21:0/a-25:0/10:0)[rac] (C59H114O6)
		2,2,2-Trichloroethanol (C2H3Cl3O)
		Ala Phe Ile Arg (C24H39N7O5)
		17beta-Nitro-5alpha-androstane (C19H31NO2)
		Phenolsulfonphthalein;Phenol red (C19H14O5S)
		CDP-DG(i-12:0/i-16:0) (C40H73N3O15P2)
		2S-Hydroxytetradecanoic acid; 2S-Hydroxytetradecanoate (C14H28O3)
		2,3,4,7,8,9,15,22,23,29-decahydroxy-14-(hydroxymethyl)-12,27,28,31,34-pentaoxo-13,25,32,35-tetraoxaoctacyclo[14.13.3.3(1),(2).0,(3).0,(1)(1).0(1),(2).0(1),(2).0(2),(3)(3)]pentatriaconta-1,3,5(30),6,8,10,19(24),20,22-nonaene-20-carboxylic acid (C33H22O22)
		Ethacrynic acid (C13H12Cl2O4)
		Ala Leu Val Arg (C20H39N7O5)
		Trp Ile Met (C22H32N4O4S1)
		Veatchine (C22H33NO2)
		2-Aminoheptanoate (C7H15NO2)
		PE-NMe2(20:3(5Z,8Z,11Z)/15:0) (C42H78NO8P)
		CDP-abequose; CDP-alpha-D-abequose (C15H25N3O14P2)
		Ophiopogonin A (C41H64O13)
		LysoPC(24:0) (C32H66NO7P)
		Vitamin K2(20) (C31H40O2)
		Glycinoeclepin A (C25H34O7)
		3-(2,4-Cyclopentadien-1-ylidene)pregn-4-en-20-one (C26H34O)
		Arg Leu Leu Pro Ala (C26H48N8O6)
		Ala Glu Trp (C19H24N4O6)
		3-bromo-7-Nitroindazole (C7H4BrN3O2)
		1-Methylphenanthrene (C15H12)
		Vemurafenib (PLX4032) (C23H18ClF2N3O3S)
		12alpha-(Chloromethyl)-12-hydroxy-pregn-4-ene-3,20-dione (C22H31ClO3)
		3,4,5-trihydroxy-6-({7,13,14-trihydroxy-3,10-dioxo-5-[5,6,7-trihydroxy-1-oxo-3-(1,2,3,4-

		tetrahydroxybutyl)-1H-isochromen-8-yl]-2,9-dioxatetracyclo[6.6.2.0,(1).0(1)(1),(1)]hexadeca-1(15),4(16),5,7,11,13-hexaen-6-yl}oxy)oxane-2-carboxylic acid (C33H26O23) Carteolol (C16H24N2O3) 6-Desmethoxy hormothamnione diacetate (C25H24O10) Tyr Arg Asn (C19H29N7O6) Asp Asp Ser (C11H17N3O9) Buflomedil (C17H25NO4) (1R,16Z,24E,26E,28Z)-1,18,19-trihydroxy-12-[1-(4-hydroxy-3-methoxycyclohexyl)propan-2-yl]-30-methoxy-15,17,21,23,29,35-hexamethyl-11,36-dioxa-4-azatricyclo[30.3.1.$0^{4,9}$]hexatriaconta-16,24,26,28-tetraene-2,3,10,14,20-pentone (C50H77NO13) Tobramycin;Nebramycin factor 6; 3'-Deoxykanamycin B (C18H37N5O9) 3,16-DIDEOXYMEXICANOLIDE-3 -DIOL (C27H36O7) Nanchangmycin (C47H78O14.Na) alpha,beta-Dihydroxyethyl-TPP;alpha,beta-Dihydroxyethyl-ThDP;2-(1,2-Dihydroxyethyl)-TPP (C14H23N4O9P2S) 2,3-Dinor-8-isoprostaglandin-F2 (C18H30O5) Phytic acid; Phytate;myo-Inositol hexakisphosphate; 1D-myo-Inositol 1,2,3,4,5,6-hexakisphosphate; D-myo-Inositol 1,2,3,4,5,6-hexakisphosphate; myo-Inositol 1,2,3,4,5,6-hexakisphosphate; Inositol 1,2,3,4,5,6-hexakisphosphate; 1D-myo-Inositol hexakisphosphate (C6H18O24P6) Immunomycin (C43H69NO12) Fludarabine (C10H13FN5O7P) 1,4-Dichlorobenzene; p-Dichlorobenzene (C6H4Cl2) Mycolactone E (C43H70O8) N-Acetyl-leu-leu-leu-leu-leu-tyr-amide; NAc-L5Y-amide (C41H69N7O8) Militarinone C (C26H33NO4) FAHFA(16:1(9Z)/13-O-16:0) (C32H60O4) Benzimidazole (C7H6N2) delta-3,4,5,6-Tetrachlorocyclohexene; 3,4,5,6-Tetrachlorocyclohexene (C6H6Cl4) Testosterone isocaproate (C25H38O3) PA(24:1(15Z)/15:0) (C42H81O8P) CDP-DG(i-12:0/i-20:0) (C44H81N3O15P2) Voacamine; Methyl-12-methoxy-13-(17-methoxy-17-oxovobasan-3alpha-yl)ibogamine-18-carboxylate (C43H52N4O5) Glycerol tricaprylate (C27H50O6) cyclo-Dopa-glucuronylglucoside (C21H27NO15) PGP(22:5(4Z,7Z,10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,16Z)) (C50H80O13P2) PE(P-18:1(11Z)/15:0) (C38H74NO7P) Ormosanine (C20H35N3)

		DG(14:1n5/0:0/22:2n6) (C39H70O5) Tocophersolan (C35H58O6) 15-cyclohexyl pentanor PGF2 (C21H34O5) PA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:2(13Z,16Z)) (C47H77O8P) PE-NMe2(9D5/13M5) (C50H88NO10P)

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3.4 Differential metabolites selection of *M*. barkari extracellular

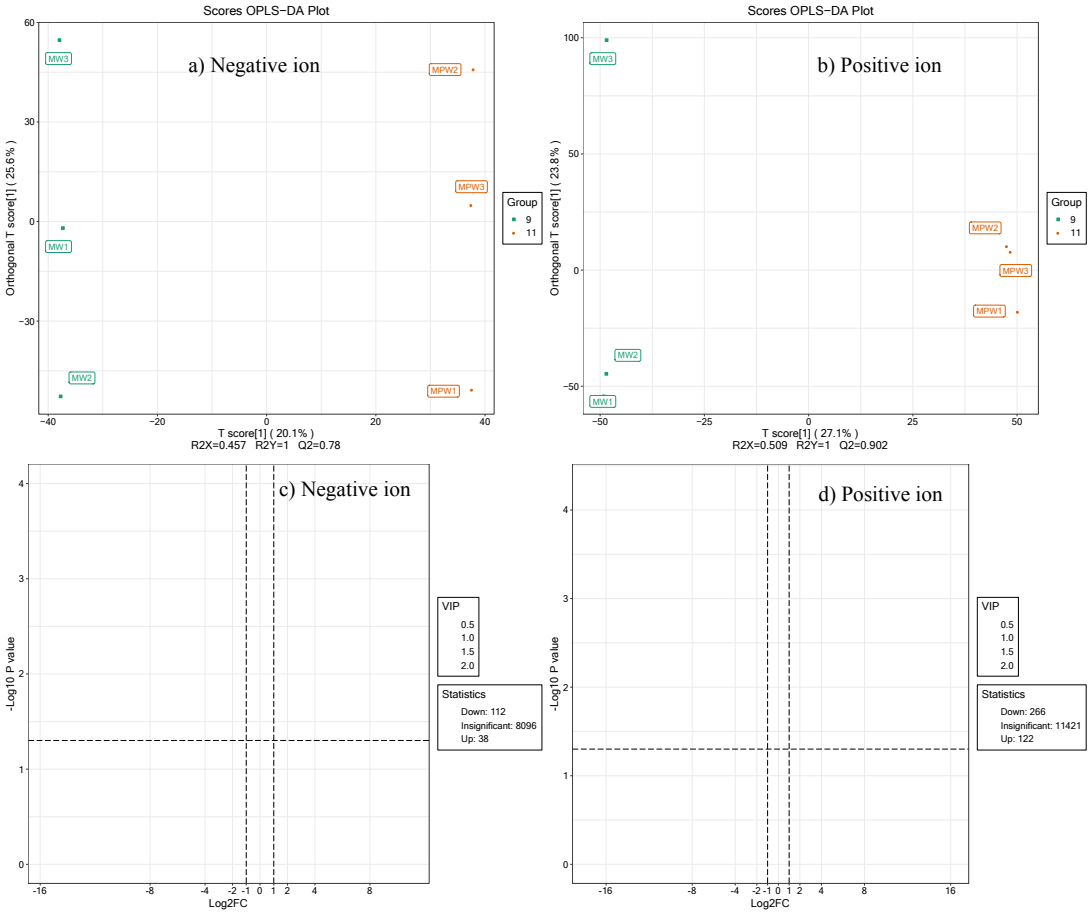

Fig. S5 OPLS_DA and volcano plots of differential metabolites of *M*. barkari extracellular

The comparison is between: with/without of γ-HCH.

291 **Table S7 Differential metabolites list of *M*. barkari extracellular between with/without γ-HCH**

Mode	Type	Intracellular
Negative	Up (24)	gamma-Glutamyltyramine (C13H18N2O4)
		FA 9 (C9H16O3)
		S-Sulfo-L-cysteine (C3H7NO5S2)
		PI(16:0/16:0) (C41H79O13P)
		PGP(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/20:2(11Z,14Z)) (C48H80O13P2)
		N-(3,4-Dichlorophenyl)-malonamate (C9H7Cl2NO3)
		PA(8:0/i-12:0) (C23H45O8P)
		TG(22:0/a-13:0/20:0)[rac] (C58H112O6)
		S-Sulfanylglutathione (C10H17N3O6S2)
		Sulfobromophthalein (C20H10Br4O10S2)
		Gliotoxin (C13H14N2O4S2)
		Methyl-CoM (C3H8O3S2)
		hydrogen trioxo[3-(1lambdachromen-1-ylium-2-yl)phenoxy]-lambdasulfanuide (C15H11O5S)
		APF (C26H17NO5)
		PS(14:0/24:0) (C44H86NO10P)
		Dimethomorph (C21H22ClNO4)
		Acetic acid, 2-[4-[[[2-[3-fluoro-4-(trifluoromethyl)phenyl]-4-methyl-5- thiazolyl]methyl]thio]-2-methylphenoxy] (C21H17F4NO3S2)
		Met Cys Asp Phe Thr (C25H37N5O9S2)
		S-1,5-Cyclohexadiene-1-carboxylate coenzymeA (C28H42N7O17P3S)
		5,7,22,24(28)-Ergostatetraenol (C28H42O)
		CL(i-14:0/i-14:0/i-12:0/i-19:0) (C68H132O17P2)
		PA(22:5(4Z,7Z,10Z,13Z,16Z)/22:0) (C47H83O8P)
		Tolytoxin (C46H75NO13)
		Levothyroxine sodium anhydrous (C15H10I4NO4.Na)
	Down (64)	7-Hydroxydodecanoate (C12H24O3)
		PA(18:2(9Z,12Z)/22:0) (C43H81O8P)
		His Ser Lys Lys (C21H38N8O6)
		Methylphosphonate (CH5O3P)
		PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/24:0) (C52H90NO10P)
		PG(20:1(11Z)/18:2(9Z,12Z)) (C44H81O10P)
		JWH 200 (C25H24N2O2)
		(4E,7E,10Z,13E,16E,19E)-docosa-4,7,10,13,16,19-hexaenoic acid (C22H32O2)
		MLS001306483-01!Cytoxan6055-19-2 (C7H17Cl2N2O3P)
		Fenamiphos (C13H22NO3PS)
		PE-NMe2(14:1(9Z)/14:0) (C35H68NO8P)

		Valaciclovir (C13H20N6O4) PG(i-12:0/a-17:0) (C35H69O10P) PysoPE 16:1 (C21H42NO7P) Bergenin (C14H16O9) TG(i-22:0/a-15:0/10:0)[rac] (C50H96O6) Glu Lys Leu Glu Ala (C25H44N6O10) 4-(3,5-Diphenylcyclohexyl)phenol (C24H24O) His His His (C18H23N9O4) CL(i-14:0/a-15:0/18:2(9Z,11Z)/a-25:0)[rac] (C81H154O17P2) PE-NMe(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:5(4Z,7Z,10Z,13Z,16Z)) (C50H78NO8P) Mibefradil (C29H38FN3O3) 2-Amino-3-carboxymuconic acid semialdehyde (C7H7NO5) Myxochromide S2 (C39H56N6O8) Asp Ile Lys Asp (C20H35N5O9) PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/24:1(15Z)) (C52H88NO10P) (S)-F-Willardiine;5-Fluorowillardiine (C7H8FN3O4) Malaoxon (C10H19O7PS) N-Butyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine (C9H13N5) Glu Ile Leu (C17H31N3O6) PS(24:1(15Z)/15:0) (C45H86NO10P) 2,3,7,8-Tetrachlorodibenzodioxin (C12H4Cl4O2) Tyr Asp Arg Arg (C25H40N10O8) U-46619 Glycine methyl ester (C24H39NO5) 3,5-Dibromo-4-hydroxybenzoate (C7H4Br2O3) LYSYL-TYROSYL-LYSINE (C21H35N5O5) Lupulone (C26H38O4) Megalomicin C1 (C48H84N2O17) (1R,16Z,24E,26E,28Z)-1,18-dihydroxy-12-[3-(4-hydroxy-3-methoxycyclohexyl)prop-1-en-2-yl]-19,30-dimethoxy-15,17,21,23,29,35-hexamethyl-11,36-dioxa-4-azatricyclo[30.3.1.$0^{4,9}$]hexatriaconta-16,24,26,28-tetraene-2,3,10,14,20-pentone (C51H77NO13) Phe Tyr Leu Leu Tyr (C39H51N5O8) Leucyl-Valine (C11H22N2O3) Leu Glu Lys Glu (C22H39N5O9) SE 175 (C16H13NO6S) X-206 (C47H82O14) His Val Leu Lys (C23H41N7O5) Prinomide (C15H13N3O2) MLS001148643-01!17ALPHA-HYDROXYPROGESTERONE CAPROATE630-56-8 (C27H40O4)

		C-6 Ceramide (C24H47NO3) HexCer-NS d34:2 (C40H75NO8) Cys Arg Arg (C15H31N9O4S1) PA(22:5(4Z,7Z,10Z,13Z,16Z)/24:0) (C49H87O8P) PA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:5(4Z,7Z,10Z,13Z,16Z)) (C47H71O8P) Phe Ala Glu Lys Ile (C29H46N6O8) 17-phenyl trinor PGF2 diethyl amide (C27H41NO4) PE-NMe(22:4(7Z,10Z,13Z,16Z)/24:0) (C52H96NO8P) 2,3,6-Trichlorobenzoic acid (C7H3Cl3O2) Colubrin (C48H76O18) PE-NMe2(9D5/13M5) (C50H88NO10P) Methyllycaconitine (C37H50N2O10) PE-NMe(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:2(13Z,16Z))(C50H84NO8P) MK 886 (C27H34ClNO2S) CGP 28014 (C12H19N3O) Pyridoxal phosphate (C8H10NO6P) PE-NMe2(14:1(9Z)/24:0) (C45H88NO8P)
Positive	Up (72)	Rebeccamycin (C27H21Cl2N3O7) Hypoxanthine-9-β-D-Arabinofuranoside (C10H12N4O5) Gamma-Linolenic acid (C18H30O2) Guanine (C5H5N5O) Triiodothyronine (C15H12I3NO4) (all-E)-6'-Apo-y-caroten-6'-al (C32H42O) Nicotinic Acid Adenine Dinucleotide (C21H27N7O14P2) Glutathione (C10H17N3O6S) Clitidine 5'-phosphate; 1,4-Dihydro-4-imino-1-(5-O-phosphono-beta-D-ribofuranosyl)-3-pyridinecarboxylic acid (C11H15N2O9P) 3-Amino-2,5-dichlorobenzoic acid (C7H5Cl2NO2) Agrimol C (C36H44O12) Flunitrazepam (C16H12FN3O3) 8-hydroxy-5-methyl-5-(4-methylpent-3-en-1-yl)-3,6-dioxatricyclo[5.4.0.0(2),]undeca-1(11),7,9-triene-11-carboxylic acid (C17H20O5) 5-Hydroxy-2-oxo-4-ureido-2,5-dihydro-1H-imidazole-5-carboxylic acid ester (C5H6N4O5) LG 100268 (C24H29NO2) Diphenylmercury (C12H10Hg) His Lys Met (C17H30N6O4S1) 2-(5'-Methylthio)pentylmalic acid; 2-(5'-Methylthio)pentylmalate (C10H18O5S) Nicotinamide, N-(2-hydroxyethyl)-(C8H10N2O2)

		Destomysin;Destomycin A (C20H37N3O13)
		Methylimidazole acetaldehyde (C6H8N2O)
		FLUTRIMAZOLE (C22H16F2N2)
		PS(18:0/24:0) (C48H94NO10P)
		1,3-alpha-D-Mannosyl-(1,2-N-acetyl-alpha-D-glucosaminyl)-1,2-alpha-D-mannosyl-1,2-alpha-D-mannosyl-D-mannose (C32H55NO26)
		DG(a-25:0/a-25:0/0:0) (C53H104O5)
		beta-D-Mannosylphosphodecaprenol (C56H93O9P)
		Nicotinamide (C24H26O7)
		4-Chlorophenylacetonitrile (C8H6ClN)
		TG(a-21:0/20:0/10:0)[rac] (C54H104O6)
		Chlorphonium chloride (C19H32Cl2P.Cl)
		D-Sedoheptuiose 7-Phosphate (C7H13BaO10P)
		Myxochromid S1 (C38H54N6O8)
		Glycoperine (C19H21NO8)
		Naltriben (C26H25NO4)
		Quetiapine fumarate (Seroquel) (C46H54N6O8S2)
		11-dehydro Thromboxane B2-d4 (C20H28D4O6)
		ALFUZOSIN (C19H27N5O4)
		Carnitine C13:0 (C20H39NO4)
		Carnitine C7:1 (C14H25NO4)
		3-(4-Chlorophenyl)-2H-1-benzopyran-2-one (C15H9ClO2)
		Ethyl tiglate (C7H12O2)
		1,4-Naphthoquinone (C10H6O2)
		2-Amino-4-hydroxy-6-hydroxymethyl-7,8-dihydropteridine (C7H9N5O2)
		Myristic Acid Alkyne (C14H24O2)
		PA(i-20:0/i-22:0) (C45H89O8P)
		Se-Methyl-L-selenocysteine (C4H9NO2Se)
		Primaquine Diphosphate (C15H21N3O)
		Tetracaine hydrochloride (Pontocaine) (C15H25ClN2O2)
		Leptomycin B (C33H48O6)
		Anandamide 0-phosphate (C22H38NO5P)
		TG(i-21:0/i-22:0/13:0) (C59H114O6)
		AG-879 (C18H24N2OS)
		2,6-Dichloro-4'-biphenylol (C13H15N3O3)
		TG(a-21:0/20:0/15:0)[rac] (C59H114O6)
		2-APB (C14H16BNO)
		TG(i-20:0/15:0/15:0) (C53H102O6)

		beta-2,3,5,6-Tetrachloro-1,4-cyclohexanediol (C6H8Cl4O2) TAXOL C (C46H57NO14) TG(i-20:0/19:0/21:0) (C63H122O6) SM-17466 (C20H21N4O5S2) CAY10641 (C28H27NO6) Ethylmethylacetic acid (C5H10O2) D-myo-Inositol-1,2,5,6-tetraphosphate (C6H16O18P4) beta-Carboline;Norharman (C11H8N2) 2,3-dinor Thromboxane B1 (C18H32O6) Chlorophyll b (C55H70MgN4O6) 1D-myo-Inositol 1,3,4-trisphosphate (C6H15O15P3) 6-Hydroxy-4-methoxy-3-(3-methyl-2-butenyl)-2-(2-phenylethenyl)benzoic acid (C21H22O4) Ziram ((C3H6NS2)2.Zn) Macrocin (C45H75NO17) Ergocornine (C31H39N5O5) Cyanidin 3-O-(2-O-beta-D-glucuronosyl)-beta-D-glucoside (C27H29O17) Terbacil (C9H13ClN2O2) 2-Chlorophenylhydrazine hydrochloride (C6H7ClN2.HCl) Imibenconazole (C17H13Cl3N4S) LYCOPODINE (C16H25NO) Valnemulin (C31H52N2O5S) Squalene (C30H50) Geranylgeraniol (C20H34O) Militarinone C (C26H33NO4) PA(14:1(9Z)/24:0) (C41H79O8P) 4,4-Dimethyl-5alpha-cholesta-8,14,24-trien-3beta-ol (C29H46O) CL(i-14:0/i-14:0/a-21:0/a-13:0)[rac] (C71H138O17P2) PA(8:0/a-17:0) (C28H55O8P) gamma-L-Glutamyl-L-cysteinyl-beta-alanine (C11H19N3O6S) 6-[2-(2H-1,3-benzodioxol-5-yl)-1-carboxy-2-oxoethyl]-3,4,5-trihydroxyoxane-2-carboxylic acid (C16H16O11) Ile Lys Ala Val His (C26H46N8O6) DG(8:0/0:0/i-19:0) (C30H58O5) PA(24:1(15Z)/24:1(15Z)) (C51H97O8P) 1-(5-Phosphoribosyl)-4-(N-succinocarboxamide)-5-aminoimidazole (C12H20N5O9P) 17Z-hexacosenoic acid (C26H50O2)
	Down (66)	2-Keto-3-deoxy-D-gluconic acid (C6H10O6) 2-Octene, 3,7-dimethyl-, (Z)- (C10H20)

		Hydrocortisone caproate (C27H40O6)
		Oleamide (C18H35NO)
		N-Cyclohexylformamide (C7H13NO)
		Avermectin A1a monosaccharide (C42H62O11)
		Ivermectin B1a (C48H74O14)
		PC(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z)) (C44H76NO8P)
		Temoporfin (C44H32N4O4)
		3,6-Dihydropyridine (C5H7N)
		Arachidonoyl dopamine (C28H41NO3)
		Olaparib (C24H23FN4O3)
		Rolipram (C16H21NO3)
		CETRIMONIUM (C19H41N)
		2-Octyl dodecanol (C20H42O)
		Stearamide (C18H37NO)
		Linoleate (C18H32O2)
		(R)-10-Hydroxystearate (C18H36O3)
		LysoPA(22:5(7Z,10Z,13Z,16Z,19Z)/0:0) (C25H41O7P)
		6,8a-Seco-6,8a-deoxy-5-oxoavermectin "1a" aglycone (C34H48O7)
		4-hydroxymethyl-4-methyl-5-cholesta-8,24-dien-3-ol (C29H48O2)
		Monolinuron (C9H11ClN2O2)
		1-Oleoyl-sn-glycero-3-phosphocholine (C26H52NO7P)
		NICOTINAMIDE MONONUCLEOTIDE (C11H15N2O8P)
		Salvianin (C42H41O24)
		Muscarine (C9H20NO2)
		Moroxydine (C6H13N5O)
		Neolinustatin (C17H29NO11)
		PS(20:5(5Z,8Z,11Z,14Z,17Z)/18:3(6Z,9Z,12Z)) (C44H70NO10P)
		LPA 22:6(C25H39O7P)
		Diloxanide(C14H11Cl2NO4)
		Azelaic acid (C9H16O4)
		Gly Lys Cys (C11H22N4O4S1)
		Glu Lys Tyr Ser Asn (C27H41N7O11)
		Thapsigargin (C34H50O12)
		Choline phosphate; Phosphorylcholine (C5H15NO4P)
		Pefloxacin (C17H20FN3O3)
		Salvinorin A (C23H28O8)
		His Ala Gln Lys (C20H34N8O6)
		CL(i-14:0/a-15:0/i-13:0/i-20:0)[rac] (C71H138O17P2)

		S-Adenosylhomocysteine-d4 (C14H16D4N6O5S) OA-6129 B1 (C20H31N3O8S) TG(20:0/i-24:0/10:0) (C57H110O6) (3,4-Dimethoxyphenyl) Acetic Acid (C10H12O4) Propofol (C12H18O) CL(i-14:0/i-14:0/a-21:0/i-12:0)[rac] (C70H136O17P2) Tipranavir (C31H33F3N2O5S) Gitogenin (C27H44O4) Cetraxate benzyl ester (C24H29NO4) MLS001074901-01!erythromycin ethylsuccinate (C43H75NO16) Dicrotophos (C8H16NO5P) Prosulfocarb (C14H21NOS) CerP(d18:1/12:0) (C30H60NO6P) PE-NMe(9D3/9D3) (C42H72NO10P) Seneciphylline (C18H23NO5) Dihomo-g-Linolenic Acid-d6 (C20H28D6O2) CAY10574 (C9H10N6O) Arg Glu Leu (C17H32N6O6) 4-O-(beta-L-Arabinofuranosyl)-(2S,4S)-4-hydroxyproline (C10H17NO7) NCGC00385243-01_C12H18O4_{(1R,2R)-2-[(2Z)-5-Hydroxy-2-penten-1-yl]-3-oxocyclopentyl}acetic acid (C12H18O4) Gly Ser Asp (C9H15N3O7) Methylselenopyruvate (C4H6O3Se) 6-Acetophenazine-1-carboxylic acid (C15H10N2O3) NAC-Diketide (C15H17NO4S) Mizolastine (Mizollen) (C24H25FN6O) MLS002154105-01!Rimexolone49697-38-3 (C24H34O3) 3beta-Fluoroandrost-5-en-17beta-ol (C19H29FO) (E)-Oak lactone (C9H16O2) Diallat;Di-allate (C10H17Cl2NOS) Ser His Val Lys (C20H35N7O6) TG(i-24:0/i-14:0/8:0) (C49H94O6) 12alpha-Hydroxyamoorstatin (C28H36O10) Acetylspiramycin;Spiramycin II (C45H76N2O15) Clofentezine (C14H8Cl2N4) His Val Phe Gly Glu (C27H37N7O8) 1-Methylnaphthalene;alpha-Methylnaphthalene (C11H10) Fluvoxamine acid (C14H17F3N2O3)

		Glu Lys Tyr Leu Gly (C28H44N6O9)
		Fexaramine (C32H36N2O3)
		Oleana-1,9(11)-dien-28-oic acid, 2-cyano-3,12-dioxo- (C31H41NO4)
		ATP;Adenosine 5'-triphosphate (C10H16N5O13P3)
		Di(2-ethylhexyl) adipate (C22H42O4)
		Bekanamycin (C18H37N5O10)
		TG(i-21:0/10:0/13:0) (C47H90O6)
		Phenyl glucuronide (C12H14O7)
		Hydroxyrepaglinide (C27H36N2O5)
		Glu Met Asp (C14H23N3O8S1)
		AL 8810 isopropyl ester (C27H37FO4)
		METHIONYL-LEUCYLPHENYLALANINE (C20H31N3O4S)
		m-chlorophenylpiperazine (m-CPP) (C10H13ClN2)
		Pumiliotoxin 251D (C16H29NO)
		TG(a-21:0/i-16:0/12:0)[rac] (C52H100O6)
		Ranitidine (C13H22N4O3S)
		2,3,4,7,8,9,15,22,23,29-decahydroxy-14-(hydroxymethyl)-13,25,32,35-tetraoxaoctacyclo[14.13.3.3(1),(2).0,(3).0,(1)(1).0(1),(2).0(1),(2).0(2),(3)(3)]pentatriaconta-1,3,5(30),6,8,10,19(24),20,22-nonaene-12,27,28,31,34-pentone (C32H22O20)
		epsilon-Rhodomycin T (C30H35NO11)
		Dibenz(a,h)acridine (C21H13N)
		Tetracenomycin A2 (C23H18O8)
		Ser Ile Asn Lys (C19H36N6O7)
		LysoPC 20:5(2n isomer) (C28H49NO7P)
		2,4-Dihydroxypteridine;Lumazine (C6H4N4O2)
		Myxochromide S3 (C40H56N6O8)
		Bisphenol A dimethacrylate (C23H24O4)
		Dihydroxyfumaric acid (C4H4O6)
		Thr Val Tyr Lys Gly (C26H42N6O8)
		1-hexadecyl-glycero-3-phosphate (C19H41O6P)
		D-Glucono-1,5-lactone (C6H10O6)
		(1R,16Z,24E,26E,28Z)-1,18-dihydroxy-12-[3-(4-hydroxy-3-methoxycyclohexyl)prop-1-en-2-yl]-19,30-dimethoxy-15,17,21,23,29,35-hexamethyl-11,36-dioxa-4-azatricyclo[30.3.1.0,]hexatriaconta-16,24,26,28-tetraene-2,3,10,14,20-pentone (C51H77NO13)
		( )15-HEDE (C20H36O3)
		PE-NMe(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:0) (C50H88NO8P)
		N-Oxyclozapine (C18H19ClN4O)
		Dihydromethanophenazine (C37H52N2O)

		16(R)-AFP 07 (free acid) (C22H30F2O5)
		AM-toxin I (C23H31N3O6)
		Ethyl(E,Z)-decadienoate (C12H20O2)
		PE-NMe(22:5(4Z,7Z,10Z,13Z,16Z)/22:0) (C50H90NO8P)
		Jamaicamide A (C27H36BrClN2O4)
		CL(i-14:0/i-17:0/i-16:0/i-24:0) (C80H156O17P2)
		Nicotyrine;beta-Nicotyrine (C10H10N2)
		Dihydroneopterin triphosphate (C9H16N5O13P3)
		Neriifolin (C30H46O8)
		Diterpenoid EF-D (C27H38O7)
		Alpha-Carotene (C40H56)
		17-Ketostypolhydroperoxide (C28H40O6)
		11-deoxy-PGF1 (C20H36O4)
		Robinin (C33H40O19)
		Pipotiazine (C24H33N3O3S2)
		Lupulone/Adlupulone (C26H38O4)
		TG(i-20:0/a-17:0/i-21:0) (C61H118O6)
		Aphylline;(+)-Aphylline (C15H24N2O)
		Arotinoid acid (C24H28O2)
		dehydrocholic acid (C24H34O5)
		Pyridaphenthion (C14H17N2O4PS)
		1-Naphthaleneacetic acid sodium salt (C12H9O2.Na)
		3,3-Difluoro-17-methyl-5alpha-androstan-17beta-ol (C20H32F2O)
		PE-NMe2(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/22:5(4Z,7Z,10Z,13Z,16Z)) (C51H80NO8P)
		Diphenylmethylphosphine (C13H13P)
		TG(16:0/16:0/20:1(11Z)) (C55H104O6)
		17-O-Acetylajmaline (C22H28N2O3)
		Diallyl trisulfide (C6H10S3)
		Biuret (C2H5N3O2)
		(17alpha,23S)-Epoxy-28,29-dihydroxy-27-norlanost-8-ene-3,24-dione (C29H44O5)
		17-Methyl-3-(2,4-cyclopentadien-1-ylidene)-5alpha-androstane-17beta-ol (C25H36O)
		Fluthiacet-methyl (C15H15ClFN3O3S2)
		TG(i-20:0/i-15:0/10:0) (C48H92O6)
		Val Leu Leu Ser Cys (C23H43N5O7S)
		Thioperamide (C15H24N4S)
		Glycyl-H-1152 (C18H24N4O3S)
		Potassium cyanate (KCNO)
		TG(a-21:0/18:0/15:0)[rac] (C57H110O6)

		Carnitine C18:0 (C25H49NO4)
		Gln Asn Phe Glu (C23H32N6O9)
		PA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0) (C40H67O8P)
		Spinasaponin A (C42H66O14)
		Tyr Ile Phe (C24H31N3O5)
		3-(Hydrohydroxyphosphoryl)pyruvate (C3H5O5P)
		Willardiine (C7H9N3O4)
		MG(22:2(13Z,16Z)/0:0/0:0) (C25H46O4)
		N-Acetyl-leu-leu-leu-leu-leu-tyr-amide (C22H39NO6)
		2-Octaprenylphenol (C46H70O)
		Lys Ala Trp (C20H29N5O4)
		LTB4 dimethyl amide (C22H37NO3)
		Taurine (C2H7NO3S)
		-JWH 073 N-(3-hydroxybutyl) metabolite-d5 (C23H16D5NO2)
		3-Methylcholanthrene (C21H16)
		Atracurium (C53H72N2O12)
		TG(20:0/i-16:0/i-19:0) (C58H112O6)
		Mycinamicin II; Mirosamicin (C37H61NO13)
		TG(i-20:0/i-14:0/i-18:0) (C55H106O6)
		Terbutryne (C10H19N5S)
		7,8-Dihydroxanthopterin (C6H7N5O2)
		4-(Cytidine 5'-diphosphate) -2-C-methyl-D-erythritol (C14H25N3O14P2)
		Pronethalol;Pronetalol (C15H19NO)
		Met Phe Thr Glu Asp (C27H39N5O11S)
		Undecanedioic acid (C11H20O4)
		5-Hydroxypentanoate (C5H10O3)
		TG(20:0/i-15:0/8:0) (C46H88O6)
		CDP-DG(a-13:0/i-22:0) (C47H87N3O15P2)
		Hydroxychlorobactene (C40H54O)
		3-O-Sulfogalactosylceramide (d18:1/24:0) (C48H93NO11S)
		Isoflurophate (C6H14FO3P)
		N-Arachidonoyl Dopamine-d8 (C28H33D8NO3)
		PE-NMe2(14:1(9Z)/24:0) (C45H88NO8P)

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3.5 Metal-contained cofactors found in *M*. barkari intracellular and extracellular

Table S8 Metal-contained cofactors found in *M*. barkari intracellular and extracellular

Mode	Metal-contained cofactors	Intracellular		Extracellular	
		no pollu	pollu	no pollu	pollu
Negative	Coenzyme F430 (C42H51N6NiO13)	6939	5508	56	48
	Cobyrinate c-monamide (C45H60CoN5O13)	1174	858	2789	2243
	Cobalt-sirohydrochlorin (C42H44CoN4O16)	571	1490	128	67
	Cobalt-precorrin 7 (C44H57CoN4O14)	8554	13030	27	102
	Cobalt-precorrin 5B (C43H50CoN4O16)	331	114	1361	520
	Cobalt-precorrin 5 (C45H53CoN4O16)	667	218	1	583
	Cobalt-factor III (C43H46CoN4O16)	5032	4142	4897	4066
	Zinc protoporphyrin-9 (C34H32N4O4Zn)	1593	846	99	60
	Fe-coproporphyrin III (C36H36FeN4O8)	944	186	1	1
	Mg-2,4-Divinyl-phaeoporphyrin a5-monomethylester (C35H30MgN4O5)	1110	770	10	58
	Molybdoenzyme molybdenum cofactor (C10H12MoN5O8PS2)	975	1061	885	659
Positive	Coenzyme F430 (C42H51N6NiO13)	2519	1471	1	55
	Cob(I)inamide (C48H72CoN11O8)	3172	4919	406	2954
	Cobalt-precorrin 5A (C45H52CoN4O16)	2332	2234	1	1
	Cobalt-precorrin 5 (C45H53CoN4O16)	1594	319	1250	417
	Cobalt-precorrin 3 (C43H48CoN4O16)	1382	667	2228	331
	Cob(II)yrinic acid a,c-diamide (C45H61CoN6O12)	388	1222	446	209
	Cobalt-dihydro-precorrin 6 (C44H55CoN4O16)	2147	877	440	1159
	Magnesium protoporphyrin (C34H32MgN4O4)	10926	3972	21	873
	Zinc protoporphyrin-9 (C34H32N4O4Zn)	1205930	692030	2009750	886436
	Fe-coproporphyrin III (C36H36FeN4O8)	18613	9258	13079	10617
	Molybdoenzyme molybdenum cofactor (C10H12MoN5O8PS2)	1962	1334	626	293

Number is the average peak in LC-MS/MS for each treatment.

3.6 KEGG pathway of enriched functions

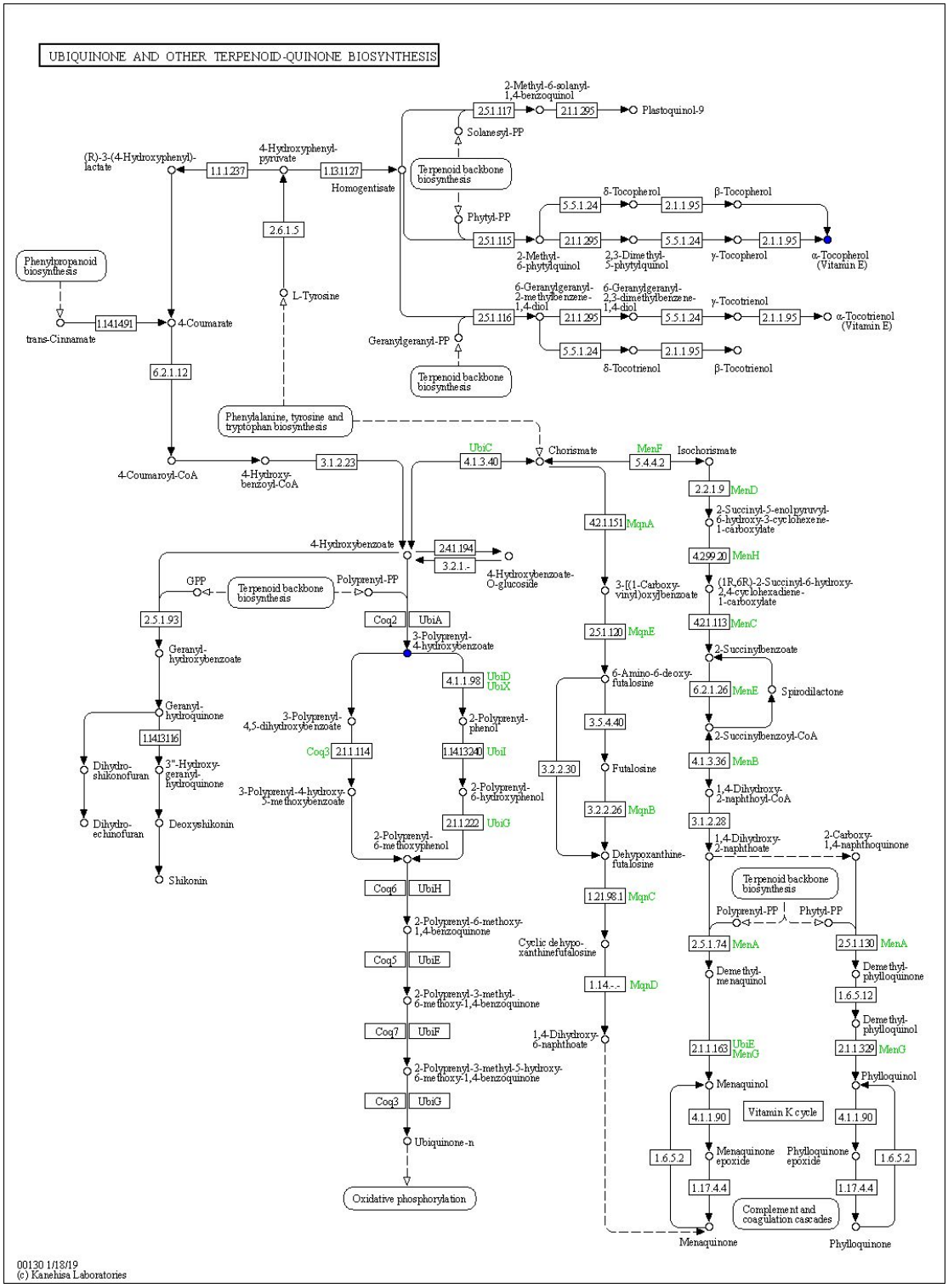


Fig. S6 Ubiquinone and other terpenoid-quinone biosynthesis (ko00130)

Red dot indicates that the metabolite is significantly up-regulated in the experimental group, and green dot indicates that the metabolite is significantly down regulated in the experimental group ($p < 0.05$).

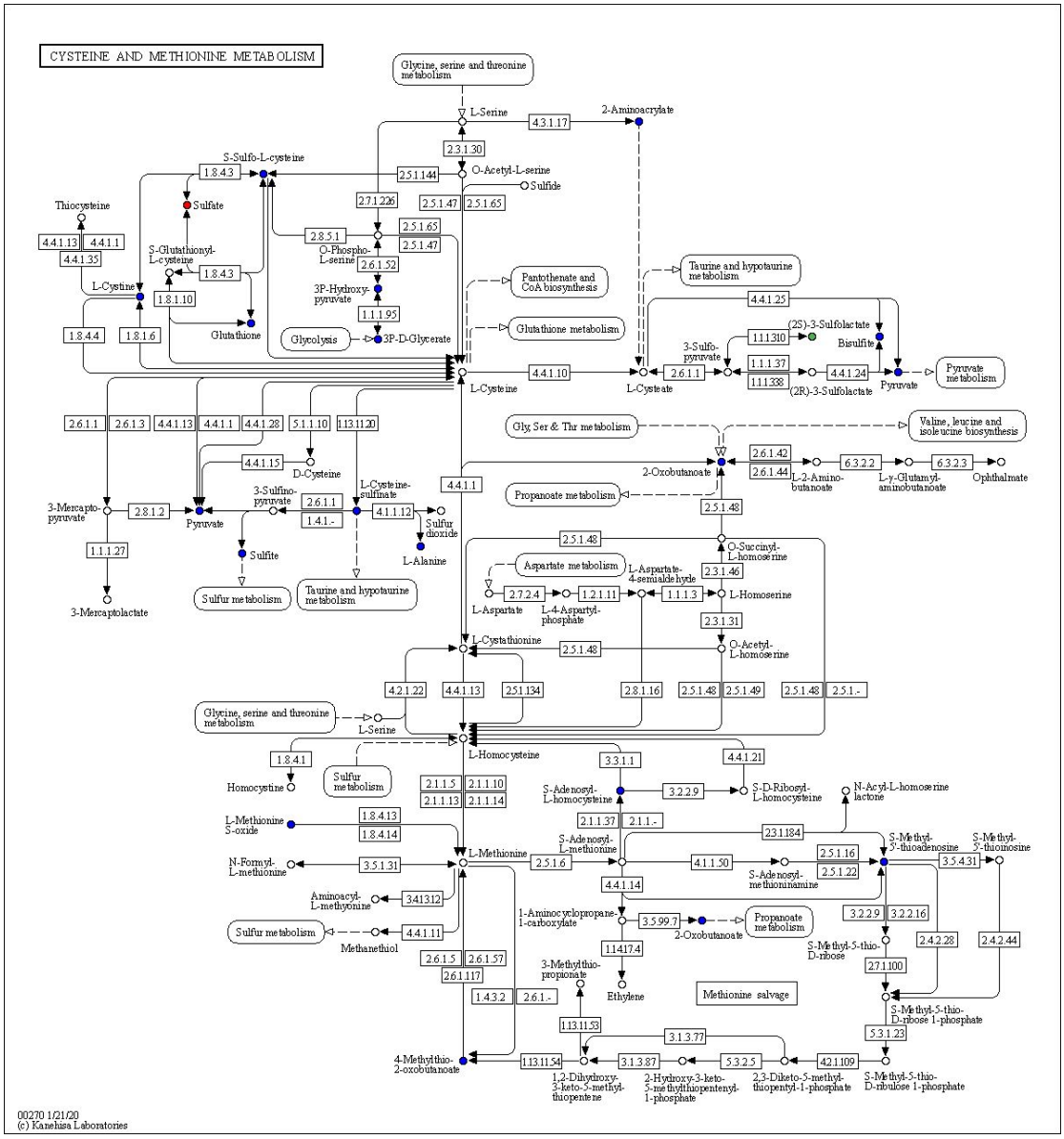


Fig. S7 Cysteine and methionine metabolism (ko00270)

Red dot indicates that the metabolite is significantly up-regulated in the experimental group, and green dot indicates that the metabolite is significantly down regulated in the experimental group ($p < 0.05$).

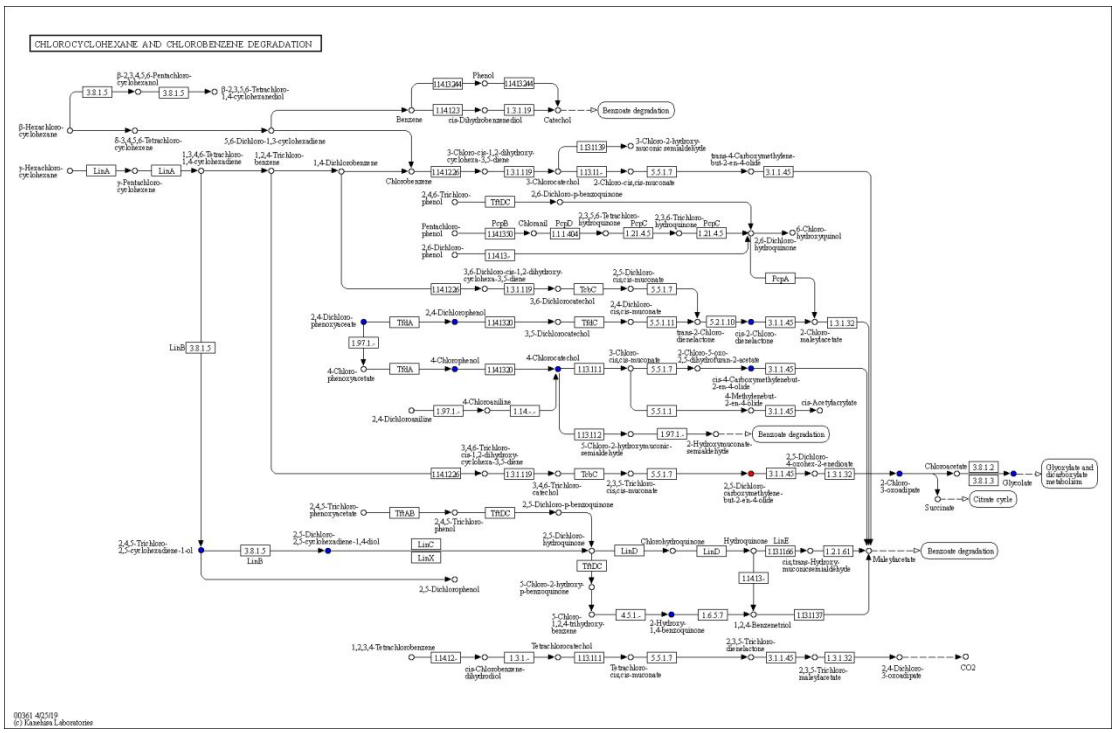


Fig. S8 Chlorocyclohexane and chlorobenzene degradation (ko00361)

Red dot indicates that the metabolite is significantly up-regulated in the experimental group, and green dot indicates that the metabolite is significantly down regulated in the experimental group ($p < 0.05$).

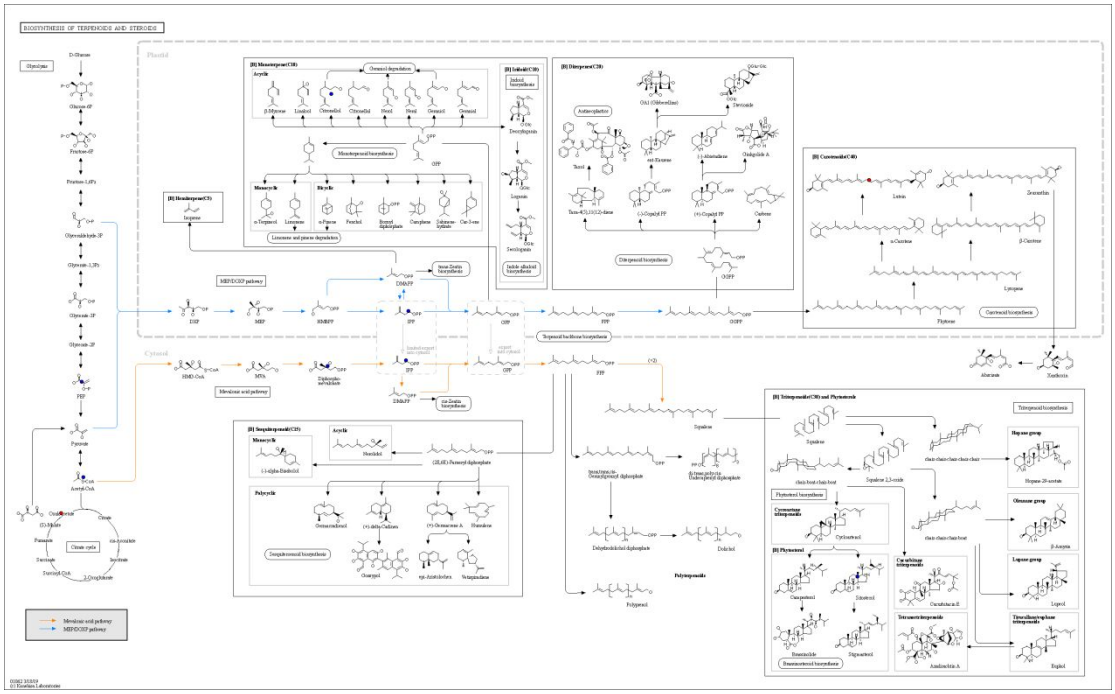


Fig. S9 Biosynthesis of terpenoids and steroids (ko01062)

Red dot indicates that the metabolite is significantly up-regulated in the experimental group, and green dot indicates that the metabolite is significantly down regulated in the experimental group ($p < 0.05$).

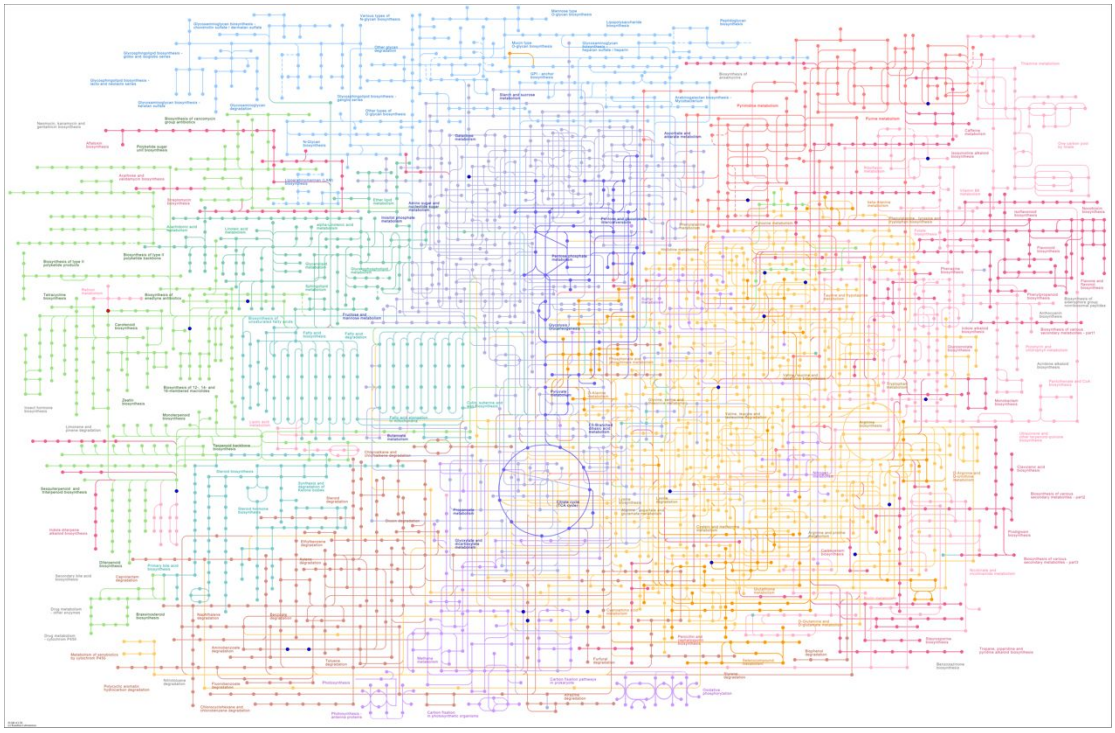


Fig. S10 Biosynthesis of secondary metabolites (Fig. S10, ko01110)

Red dot indicates that the metabolite is significantly up-regulated in the experimental group, and green dot indicates that the metabolite is significantly down regulated in the experimental group ($p < 0.05$).

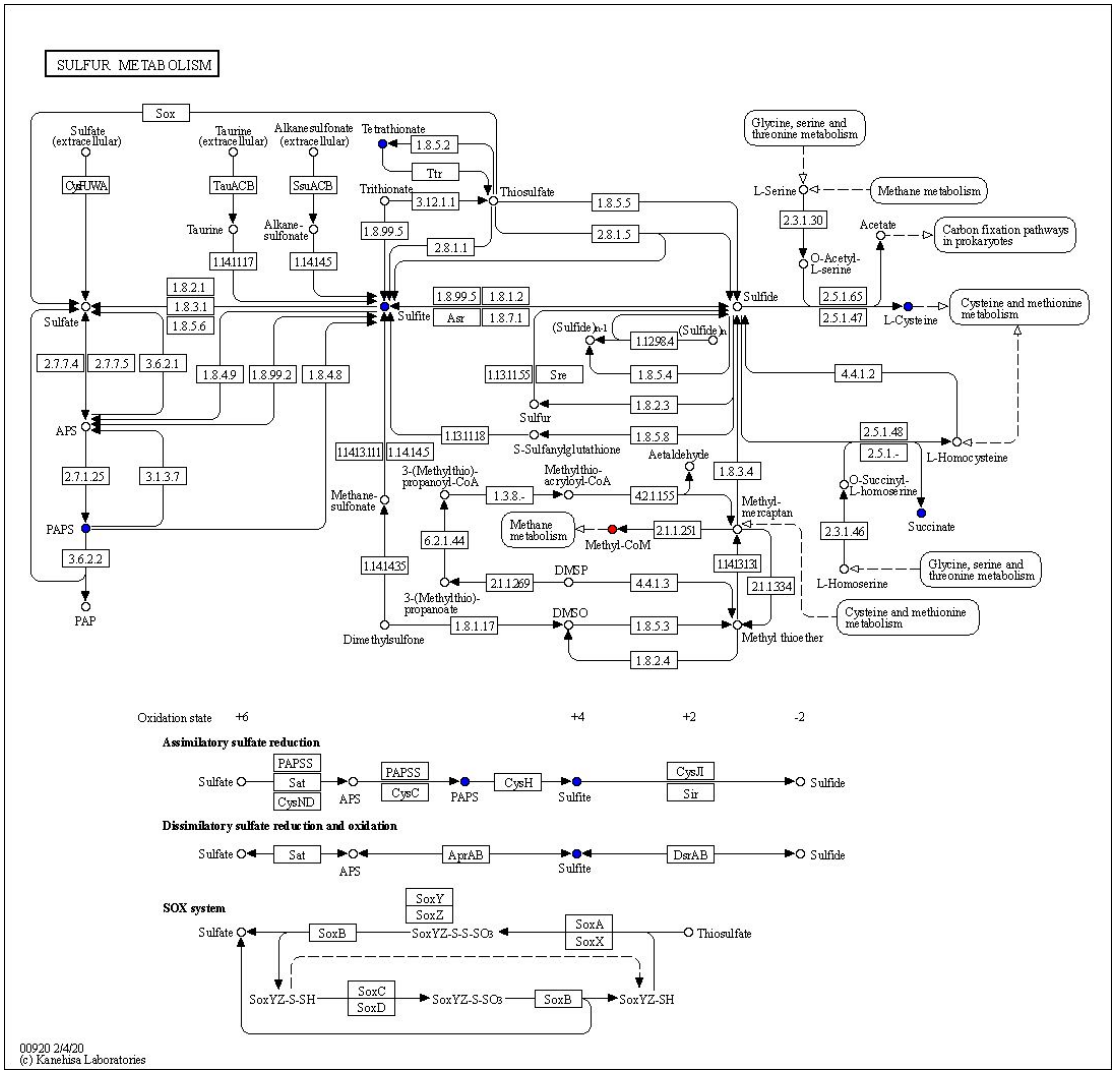


Fig. S11 Functions of sulfur metabolism (ko00920)

Red dot indicates that the metabolite is significantly up-regulated in the experimental group, and green dot indicates that the metabolite is significantly down regulated in the experimental group ($p < 0.05$).

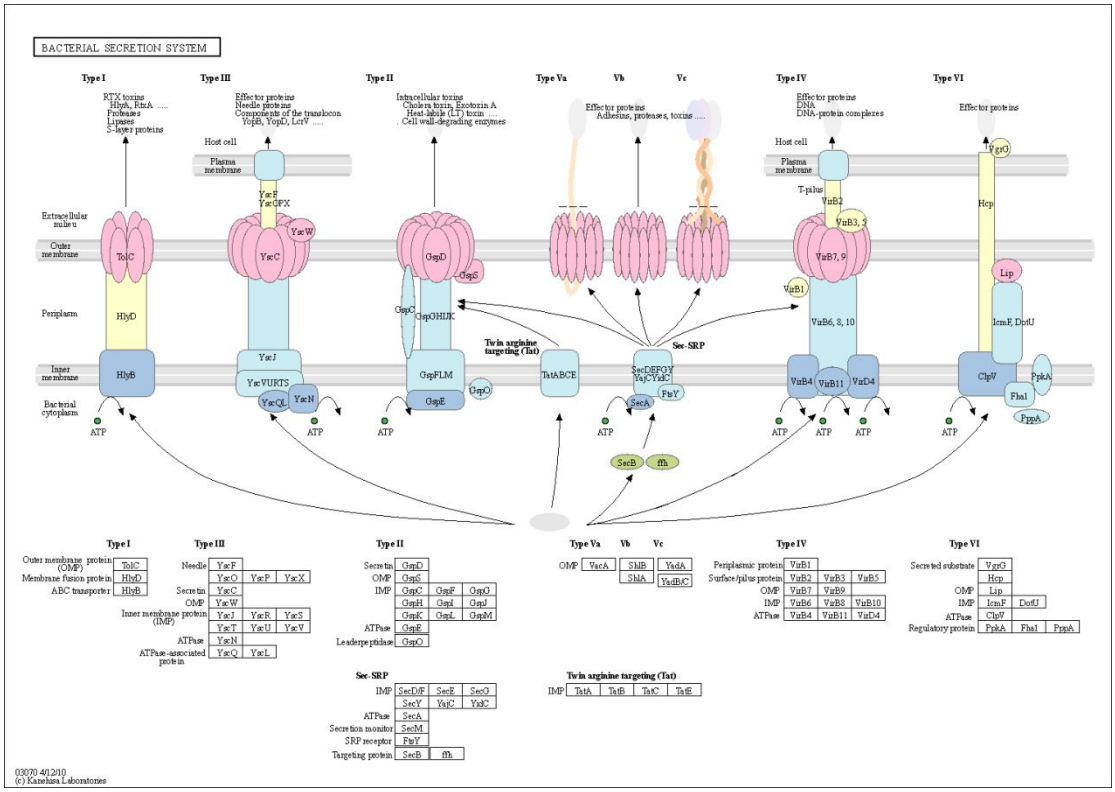


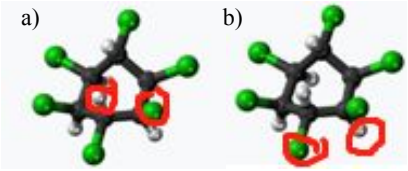
Fig. S12 Functions of bacterial secretion system (ko03070)

Red dot indicates that the metabolite is significantly up-regulated in the experimental group, and green dot indicates that the metabolite is significantly down regulated in the experimental group ($p < 0.05$).

345

346 **3.7 Transition state**

347



348 **Fig. S13 Path of the dechlorination of γ-HCH**

349 The green atom is chlorine; the grey atom is hydrogen. In Table S9, path 1 and path 2 calculated the
350 reaction energy of pathway a) and b), respectively.

351

352 **Table S9. Simulated reaction energies**

Solvent	Process	Mode	Path 1			Path 2		
			IS	TS	FS	IS	TS	FS
Vacuum	$C_6H_6Cl_6 \rightarrow C_6H_5Cl_5 + HCl$	Self	-90.41	-88.23	-90.26	-90.41	-88.46	-90.24
		F430	-808.23	-806.40	-807.89	-807.98	-806.82	-807.70
	$C_6H_5Cl_5 \rightarrow C_6H_4Cl_4 + HCl$	Self	-84.05	-81.37	-83.63	-84.01	-81.83	-83.65
		F430	-801.37	-800.21	-801.00	-801.61	-799.67	-801.16
Soil	$C_6H_6Cl_6 \rightarrow C_6H_5Cl_5 + HCl$	Self	-90.58	-88.61	-90.43	-90.58	-88.73	-90.40
		F430	-810.13	-808.94	-809.87	-809.89	-808.40	-809.77
	$C_6H_5Cl_5 \rightarrow C_6H_4Cl_4 + HCl$	Self	-84.18	-81.76	-83.79	-84.16	-82.10	-83.78
		F430	-803.38	-802.72	-803.15	-803.55	-802.21	-803.21
Water	$C_6H_6Cl_6 \rightarrow C_6H_5Cl_5 + HCl$	Self				-90.68	-88.86	-90.50
		F430				-810.56	-809.24	-810.50
	$C_6H_5Cl_5 \rightarrow C_6H_4Cl_4 + HCl$	Self				-84.24	-82.21	-83.86
		F430				-804.21	-803.08	-803.89

353 IS, initial state; TS, transition state; FS, final state. Self, self-dissociation; F430, F430-catalyzed
354 dechlorination. Since the energy barriers between path 1 and path 2 were no significantly different
355 in vacuum and soil, we then only modified the energy of path 2 in water solvent.

356

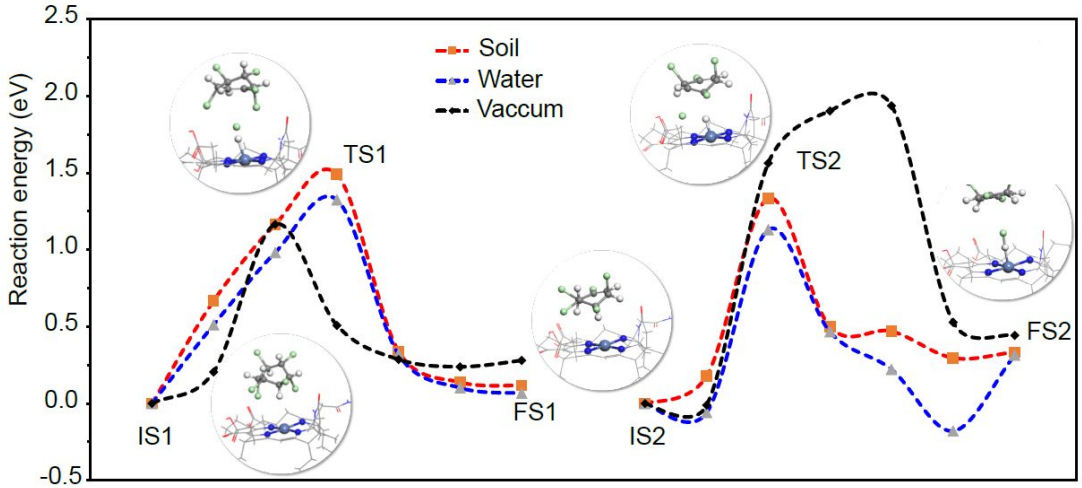


Fig. S14. Reaction energies of the transition states for F430-catalyzed dechlorination

The curves show how the transition states were corrected step-by-step in the Gaussian and Vienna *ab initio* simulation package (VASP). The Perdew-Burke-Ernzerhof (PBE) functional was used with a cut-off energy of 400 eV. IS1, initial state, which is γ-HCH ($H_6C_6Cl_6$). TS1, transition state for $H_6C_6Cl_6$ to transform to $H_6C_6Cl_5$. FS1, final state, which is $H_6C_6Cl_5$. IS2, initial state, which is $H_6C_6Cl_5$. TS2, transition state for $H_6C_6Cl_5$ to transform to $H_6C_6Cl_4$. FS2, final state, which is $H_6C_6Cl_4$.

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