

## *Supporting Information*

*for*

### **Insights into antimicrobial agent sulfacetamide transformation during chlorination disinfection process in aquaculture water**

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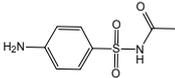
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**Table S1 Physical/chemical properties of SFA**

CAS number	Formula	Chemical structure	Molecule weight (g/mol)	Solubility in water (mg/L)	pKa <sub>1</sub>	pKa <sub>2</sub>
144-80-9	C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> SO <sub>3</sub>		214.24200	<0.01 g/100 mL at 16 °C	1.76±0.04	5.22±0.01

### Text S1

The organic intermediates formed during the SFA degradation were identified with the samples pretreated by liquid-liquid extraction (using CH<sub>2</sub>Cl<sub>2</sub> solvent) to extract and concentrate compounds of different polarity and volatility. Spectra were obtained with a gas chromatography-mass spectrometry (Shimadzu GCMS-QP2010 plus), equipped with DB-5 column (30 m×0.32 mm×0.25 μm), interfaced directly to the mass spectrometer used as a detector. The injections were made in the splitless mode using an injection temperature of 250 °C and the injection volume was 1 uL. Helium was used as carrier gas. The GC column was operated in a temperature programmed mode with an initial temperature of 40 °C held for 5 min, ramp first to 100 °C with a 15 °C/min rate, then to 200 °C with 5 °C/min rate, and then to 270 °C with 20 °C/min rate and held at that temperature for 5 min. Mass spectra were recorded in electron ionization (EI) mode at an ion source temperature of 230 °C and an electron energy of 70 eV. The mass range scanned was 30-400 m/z. The substance analysis was undertaken with reference to the NIST05 mass spectral library database.

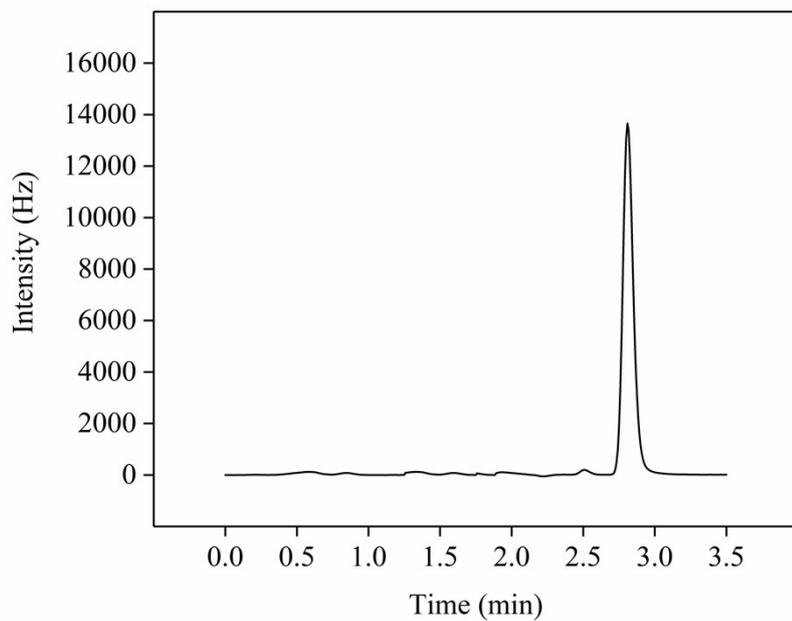


Fig. S1 The HPLC chromatogram map of SFA. Experimental conditions:  $[SFA]_0 = 5 \text{ mg/L}$ ,  $\text{pH}_{\text{ini}} = 5$ .

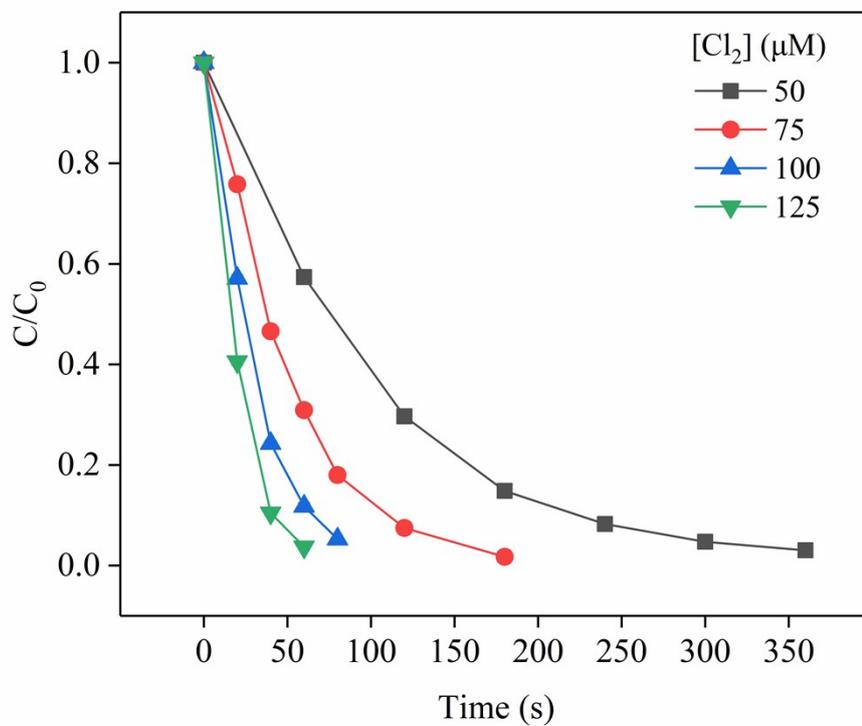


Fig. S2 Effect of  $[Cl_2]$  dose. Experimental conditions:  $[SFA]_0 = 5 \text{ μM}$ ,  $\text{pH}_{\text{ini}} = 5$ ,  $T = 20 \text{ °C}$ .

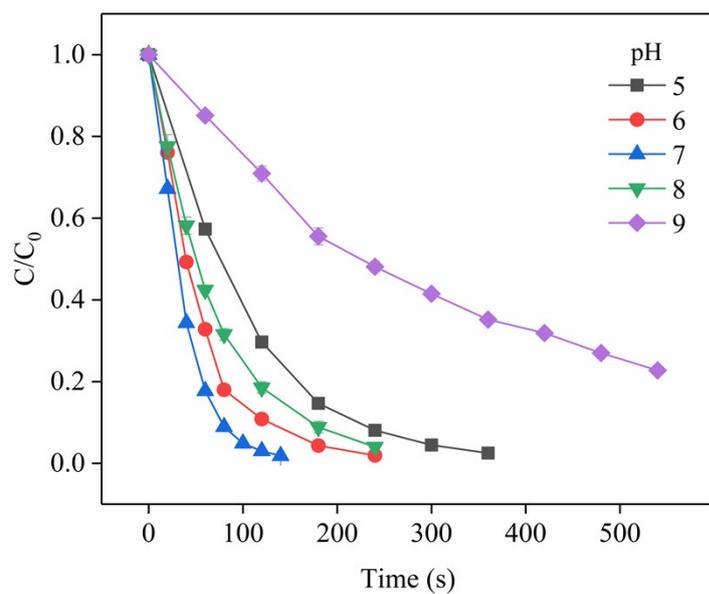


Fig. S3 Oxidation of SFA by  $[Cl_2]$  at different pH values. Experimental conditions:  $[SFA]_0 = 5 \mu M$ ,  $[Cl_2]_0 = 50 \mu M$ ,

$T = 20 \text{ }^\circ C$ .

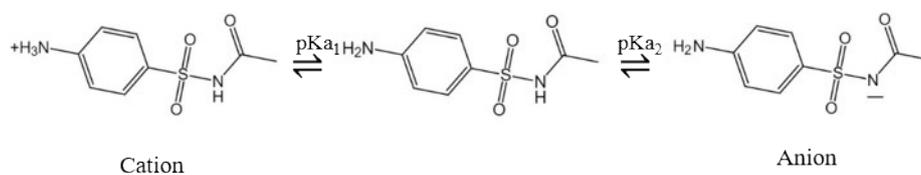


Fig.S4. Speciation patterns of SFA.

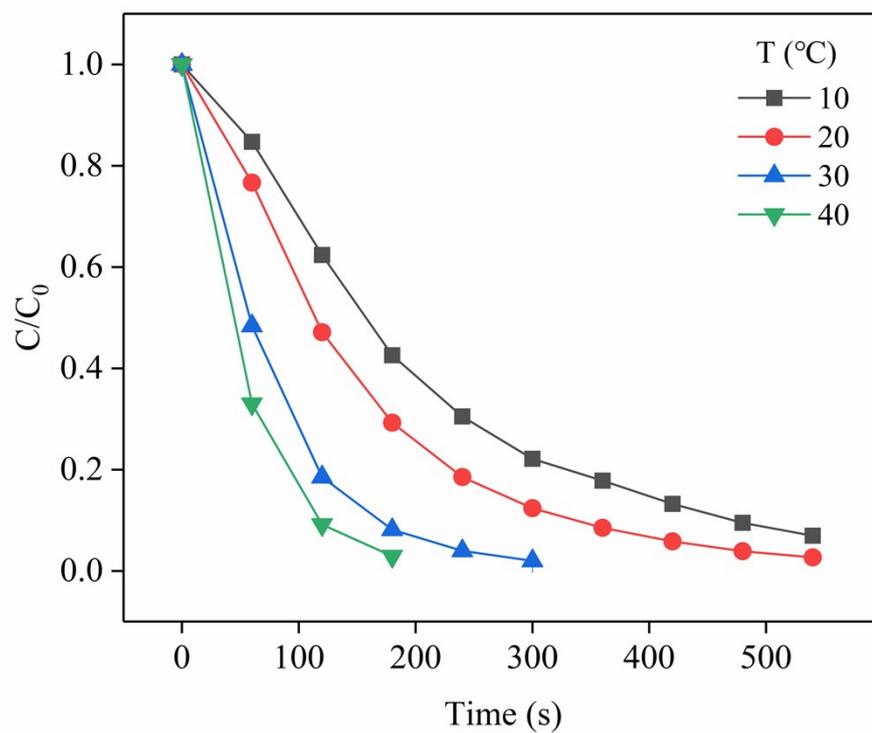


Fig. S5 Effect of water temperature. Experimental conditions:  $[SFA]_0 = 5 \mu\text{M}$ ,  $[Cl_2]_0 = 50 \mu\text{M}$ ,  $\text{pH}_{\text{ini}} = 5$ .

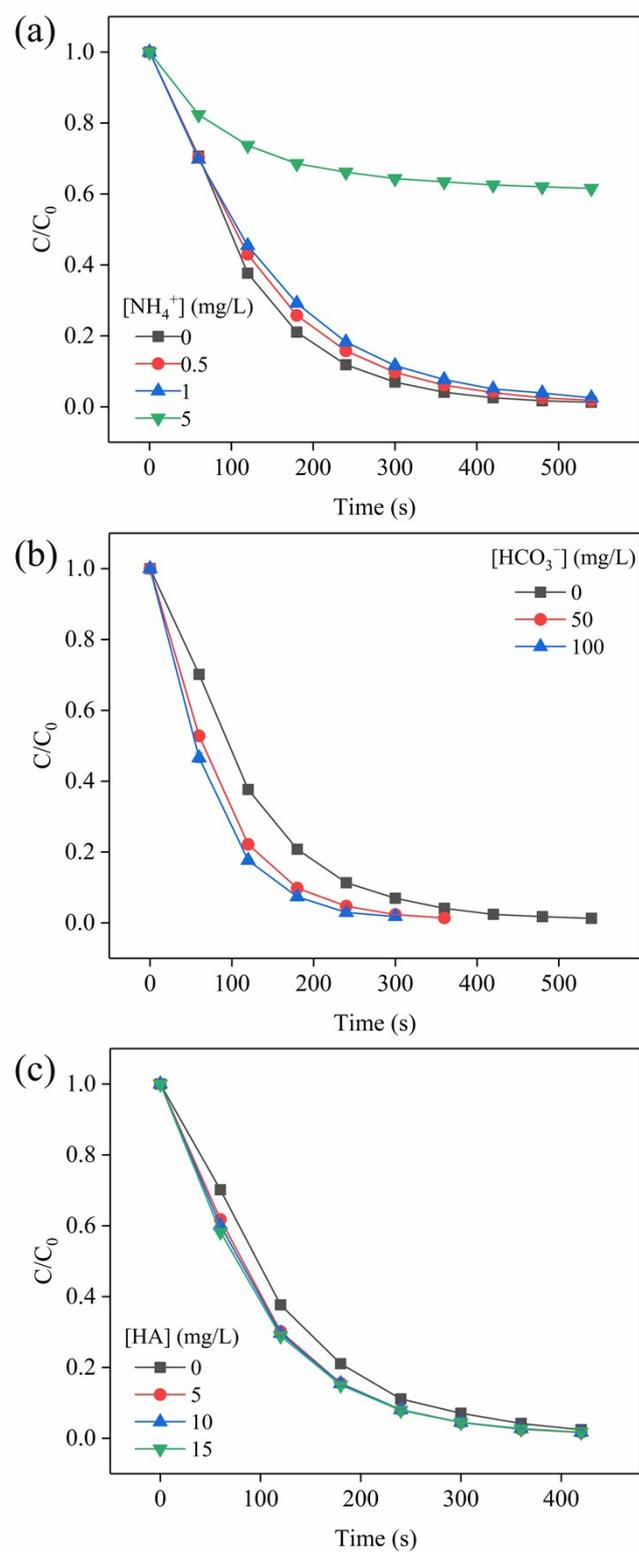


Fig. S6 Effects of concentrations of (a)  $\text{NH}_4^+$ , (b)  $\text{HCO}_3^-$ , and (c) HA on the oxidation of SFA by  $[\text{Cl}_2]$ .

Experimental conditions:  $[\text{SFA}]_0 = 5 \mu\text{M}$ ,  $[\text{Cl}_2]_0 = 50 \mu\text{M}$ ,  $\text{pH}_{\text{ini}} = 5$ ,  $T = 20 \text{ }^\circ\text{C}$ .

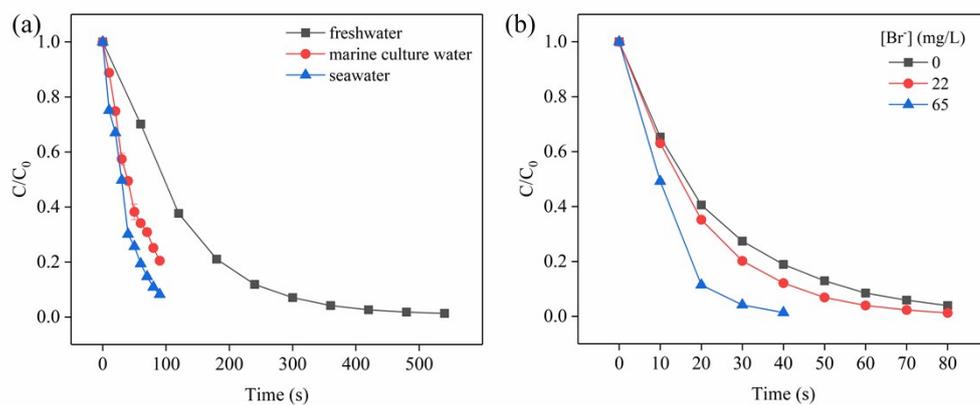


Fig. S7 Effects of (a) different water bodies and (b)  $Br^-$  concentration on SFA degradation. Experimental conditions:  $[SFA]_0 = 5 \mu M$ ,  $[Cl_2]_0 = 50 \mu M$ ,  $pH_{ini} = 5$ ,  $T = 20 \text{ }^\circ C$ .

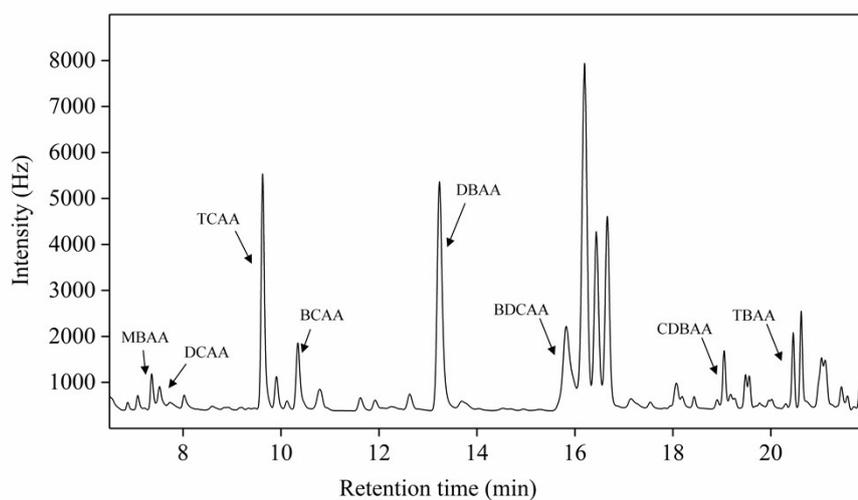


Fig. S8 GC chromatogram of the reaction products after methyl esterification pretreatment in the simulated seawater. Note: Chromatogram of HAAs corresponding to methylated products.

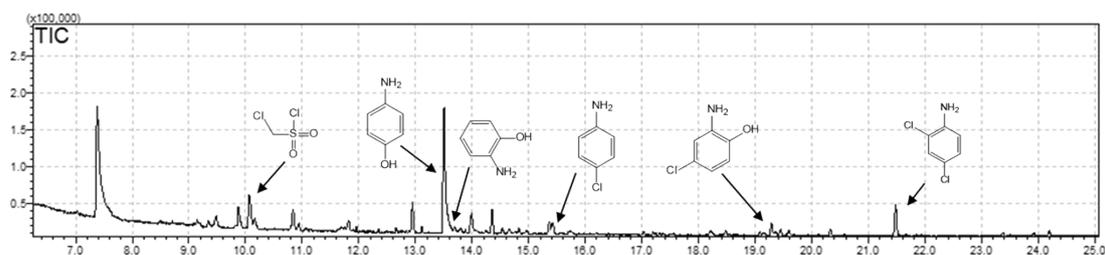


Fig. S9 The total ion chromatogram of the sample after SFA degradation for 2 min in  $NaClO$  system.

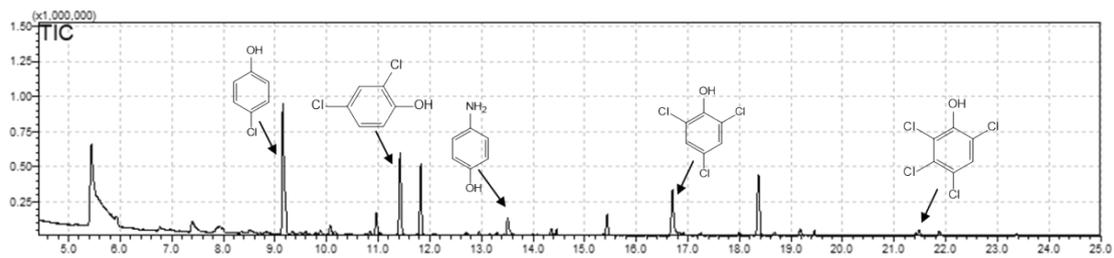


Fig. S10 The total ion chromatogram of the sample after SFA degradation for 90 min in NaClO system.

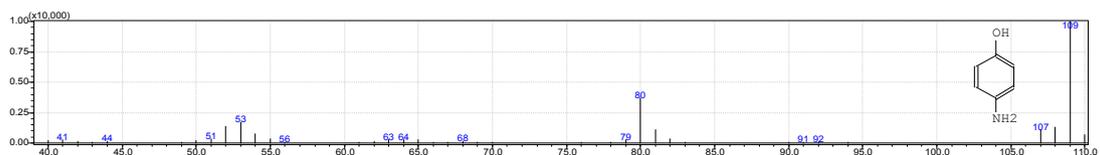


Fig.S11 The GC-MS spectrum of P-aminophenol.

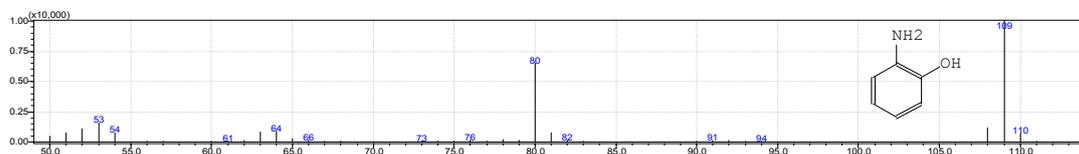


Fig.S12 The GC-MS spectrum of 2-hydroxyaniline.

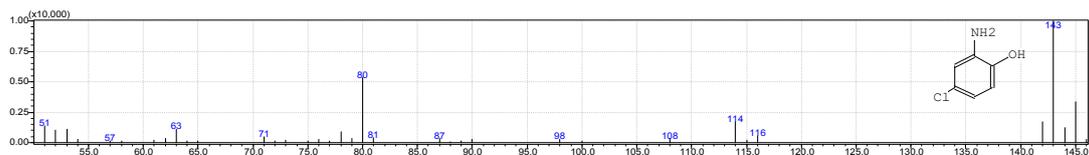


Fig.S13 The GC-MS spectrum of 2-amino-4-chlorophenol.

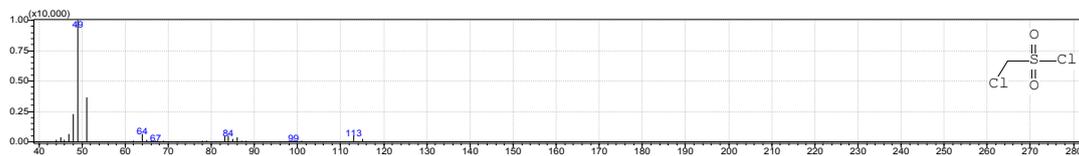


Fig.S14 The GC-MS spectrum of CH<sub>2</sub>SO<sub>2</sub>Cl<sub>2</sub>

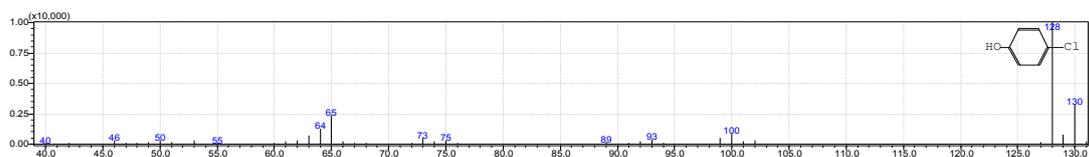


Fig.S15 The GC-MS spectrum of 4-chlorophenol.

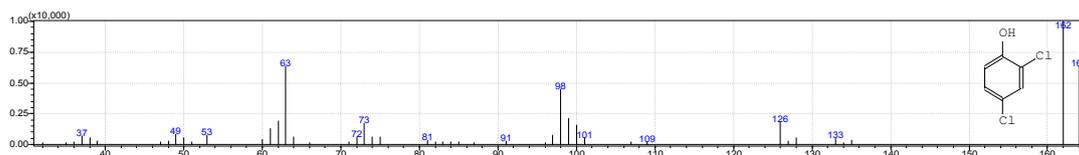


Fig.S16 The GC-MS spectrum of 2,4-dichlorophenol.

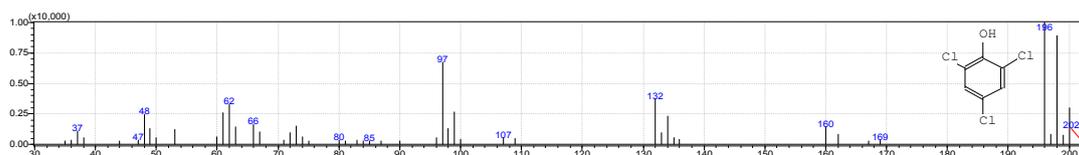


Fig.S17 The GC-MS spectrum of 2,4,6-trichlorophenol.

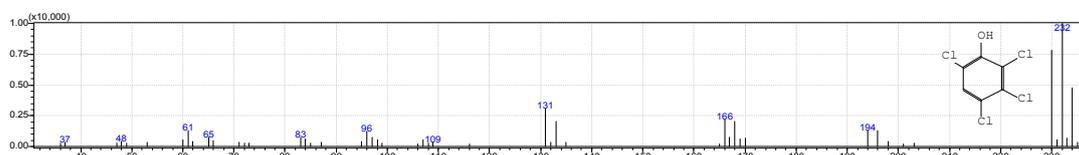


Fig.S18 The GC-MS spectrum of 2,3,4,6-tetrachlorophenol.

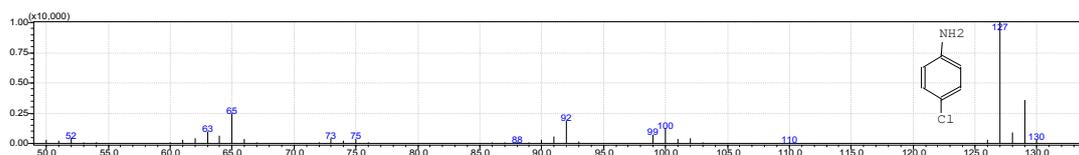


Fig.S19 The GC-MS spectrum of 4-Chloroaniline.

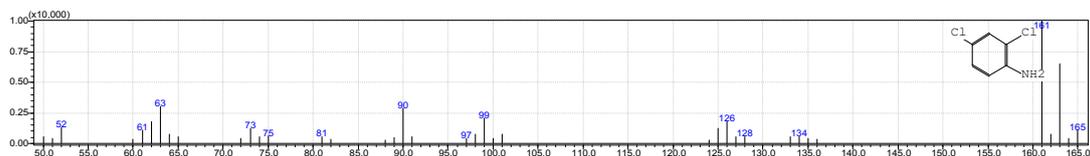


Fig.S20 The GC-MS spectrum of 2,4-dichloroaniline.