Gas Chromatography / Mass Spectrometry analysis of reaction products of sulfur mustards with phenol

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SUPPLEMENTARY INFORMATION

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Table S1. HRMS data of the typical ions detected in the EI mass spectra of compounds **1-7**.

Compound No.	**ion (*m/z*)**	**Elemental composition**	**Observed mass (*m/z*)**	**Calculated mass (*m/z*)**	**Error (in ppm)**
1	274	$C_{16}H_{18}SO_2$	274.1032	274.1028	1.48
	181	$C_{10}H_{13}SO$	181.0690	181.0687	1.70
	153	C_8H_9SO	153.0368	153.0374	-3.83
	125	C_6H_5SO	125.0067	125.0061	4.91
	121	C_8H_9O	121.0643	121.0653	-8.39
	107	C_7H_7O	107.0491	107.0497	-5.62
	94	C_6H_6O	94.0412	94.0419	-6.59
2	306	$C_{16}H_{18}S_2O_2$	306.0733	306.0748	-4.91
	213	$C_{10}H_{13}S_2O$	213.0416	213.0408	3.85
	185	$C_9H_{13}S_2$	185.0454	185.0459	-2.54
	157	$C_6H_5S_2O$	156.9789	156.9782	4.46
	153	C_8H_9SO	153.0382	153.0374	4.87
	137	C_7H_5SO	137.0062	137.0061	0.68
	125	C_6H_5SO	125.0061	125.0061	-0.26
3	320	$C_{17}H_{20}S_2O_2$	320.0904	320.0905	-0.10
	227	$C_{11}H_{15}S_2O$	227.0560	227.0564	-1.91
	199	$C_9H_{11}S_2O$	199.0247	199.02513	-2.25
	167	$C_9H_{11}SO$	167.0523	167.0531	-4.40
	153	C_8H_9SO	153.0373	153.0374	-0.83
	139	C_7H_7SO	139.0214	139.0218	-2.59
4	334	$C_{18}H_{22}S_2O_2$	334.1050	334.1061	-3.31
	241	$C_{12}H_{17}S_2O$	241.0706	241.0721	-6.02
	240	$C_{12}H_{16}S_2O$	240.0627	240.0643	-6.66
	213	$C_{10}H_{13}S_2O$	213.0414	213.0408	2.89
	181	$C_{10}H_{13}SO$	181.0689	181.0687	1.02
	157	$C_6H_5S_2O$	156.9785	156.9782	1.99
	153	C_8H_9SO	153.0381	153.0374	4.43
	147	$C_6H_{11}S_2$	147.0309	147.0302	4.53
	125	C_6H_5SO	125.0059	125.0061	-1.48
	121	C_8H_9O	121.0648	121.0653	-4.54
5	348	$C_{19}H_{24}S_2O_2$	334.1050	334.1061	-3.31
	254	$C_{16}H_{18}O_2S_2$	306.0733	306.0748	-4.91
	227	$C_{11}H_{15}S_2O$	227.0560	227.0564	-1.91
	195	$C_{11}H_{15}SO$	195.0843	195.0844	-0.31
	157	$C_6H_5S_2O$	156.9781	156.9782	-0.80
	133	C_5H_9SO	133.0141	133.0146	-3.63
	125	C_6H_5SO	125.0068	125.0061	5.67
	121	C_8H_9O	121.0650	121.0653	-3.05
6	362	$C_{20}H_{26}S_2O_2$	362.1374	362.1374	-0.17
	268	$C_{14}H_{20}S_2O_2$	268.0962	268.0956	2.41
	241	$C_{12}H_{17}S_2O$	241.0720	241.0721	-0.51
	209	$C_{12}H_{17}SO$	209.1002	209.1000	0.90
	153	C_8H_9SO	153.0370	153.0374	-2.62
	147	$C_6H_{11}S_2$	147.0295	147.0302	-4.70
	125	C_6H_5SO	125.0057	125.0061	-3.41
	121	C_8H_9O	121.0651	121.0653	-2.28
7	376	$C_{21}H_{28}S_2O_2$	376.1514	376.1531	-4.34
	283	$C_{15}H_{23}S_2O$	283.1198	283.1190	2.80
	282	$C_{15}H_{22}S_2O$	282.1128	282.1112	5.67
	255	$C_{13}H_{19}S_2O$	255.0866	255.0877	-4.57
	223	$C_{13}H_{19}SO$	223.1188	223.1190	-1.01
	189	$C_9H_{17}S_2$	189.0782	189.0772	5.08

	161	$C_7H_{13}S_2$	161.0456	161.0459	-1.80
	153	C_8H_9SO	153.0367	153.0374	-4.94
	129	$C_7H_{13}S$	129.0744	129.0738	4.40
	125	C_6H_5SO	125.0053	125.0061	-6.62
	121	C_8H_9O	121.0657	121.0653	3.25

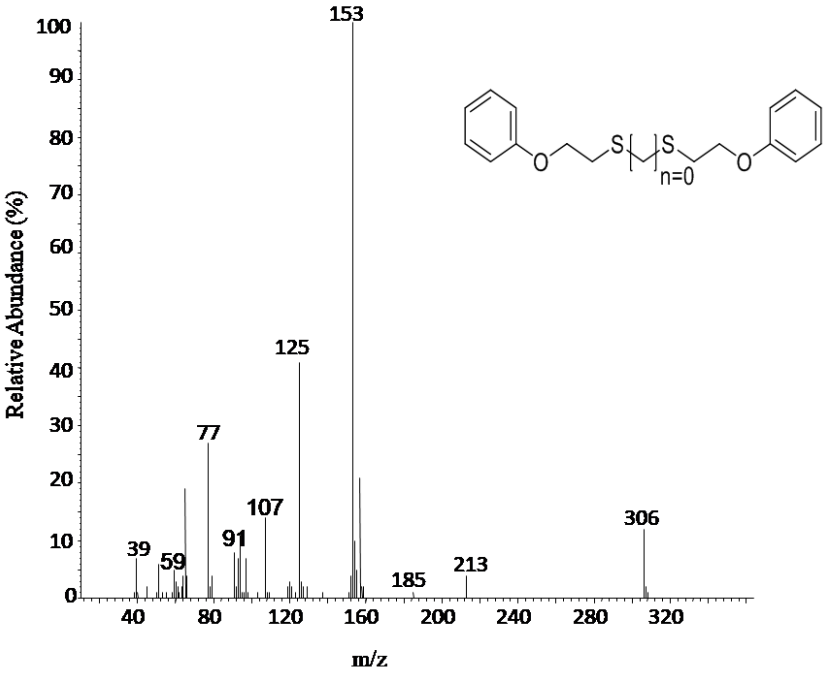

Figure S1. EI mass spectrum of compound 2.

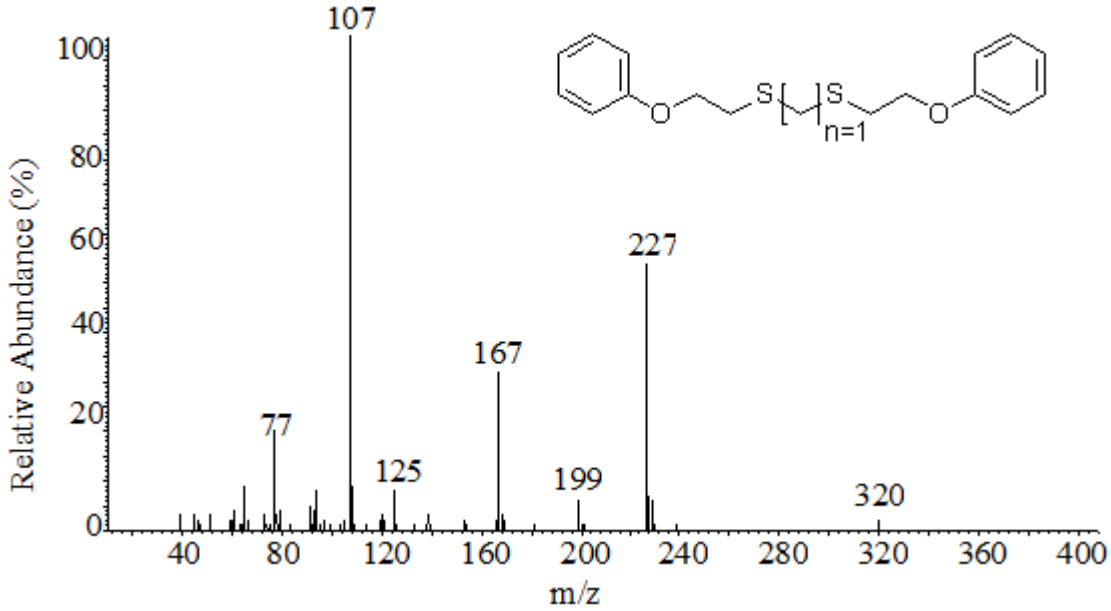

Figure S2. EI mass spectrum of compound 3.

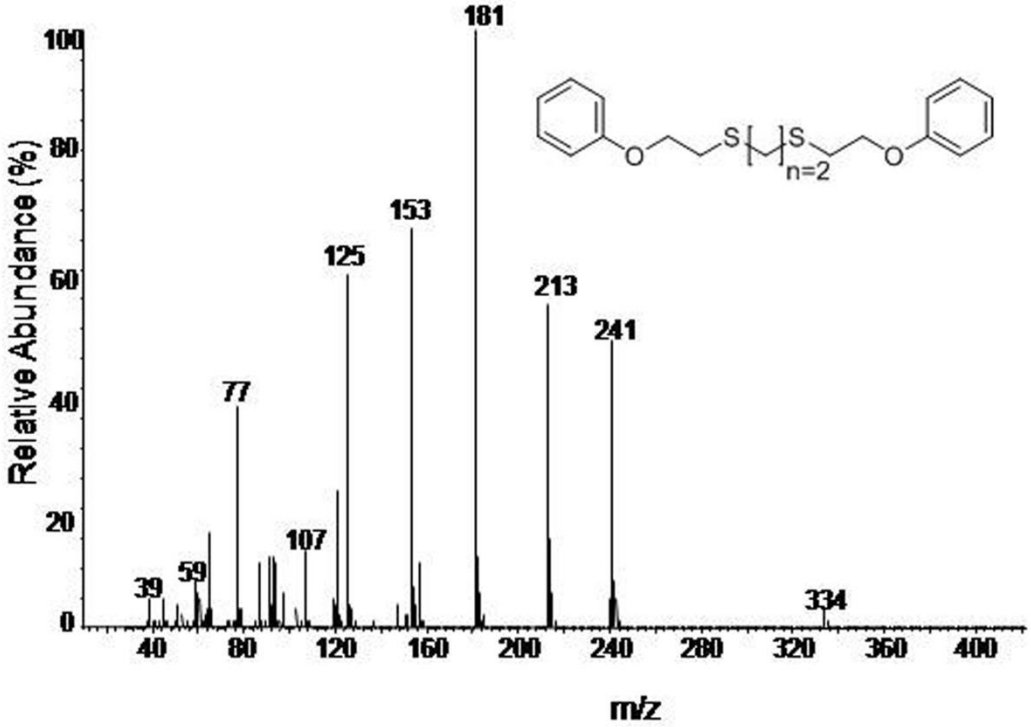

Figure S3. EI mass spectrum of compound 4.

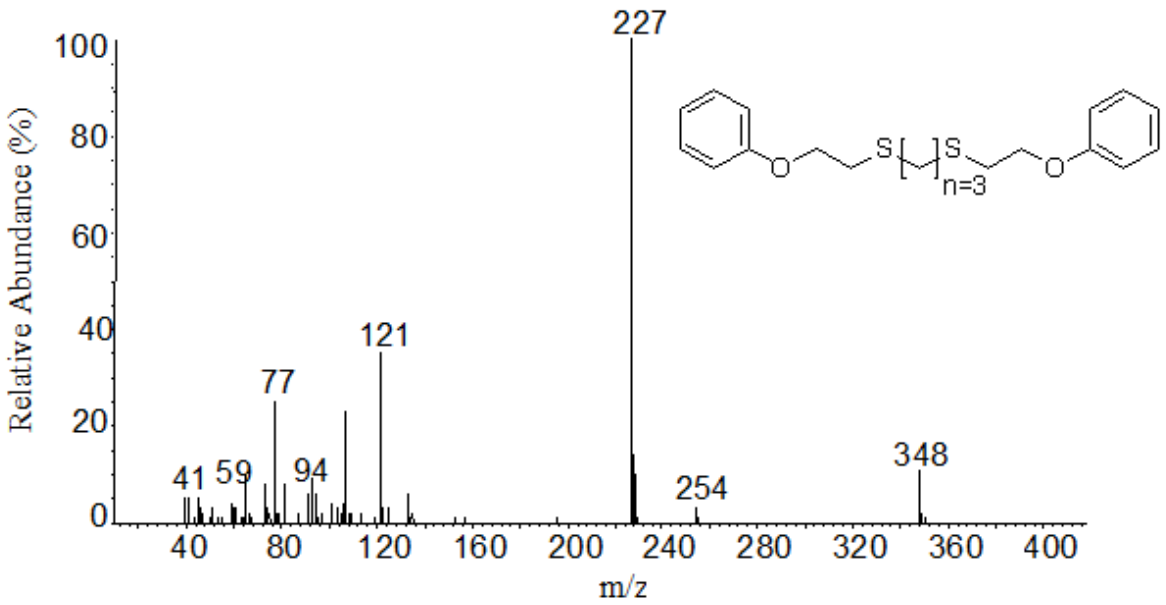

Figure S4. EI mass spectrum of compound 5.

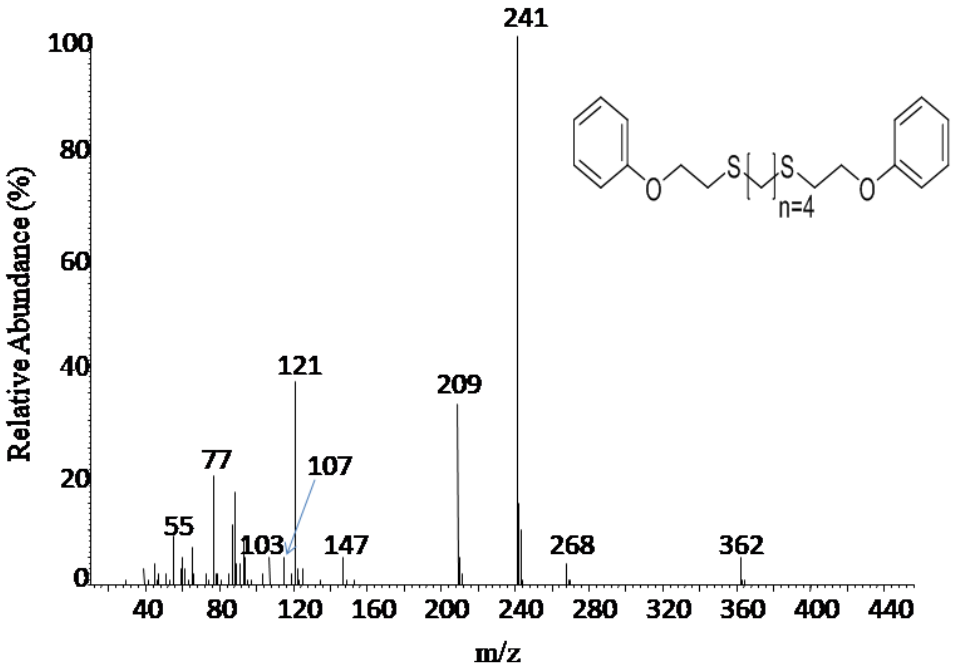

Figure S5. EI mass spectrum of compound 6.

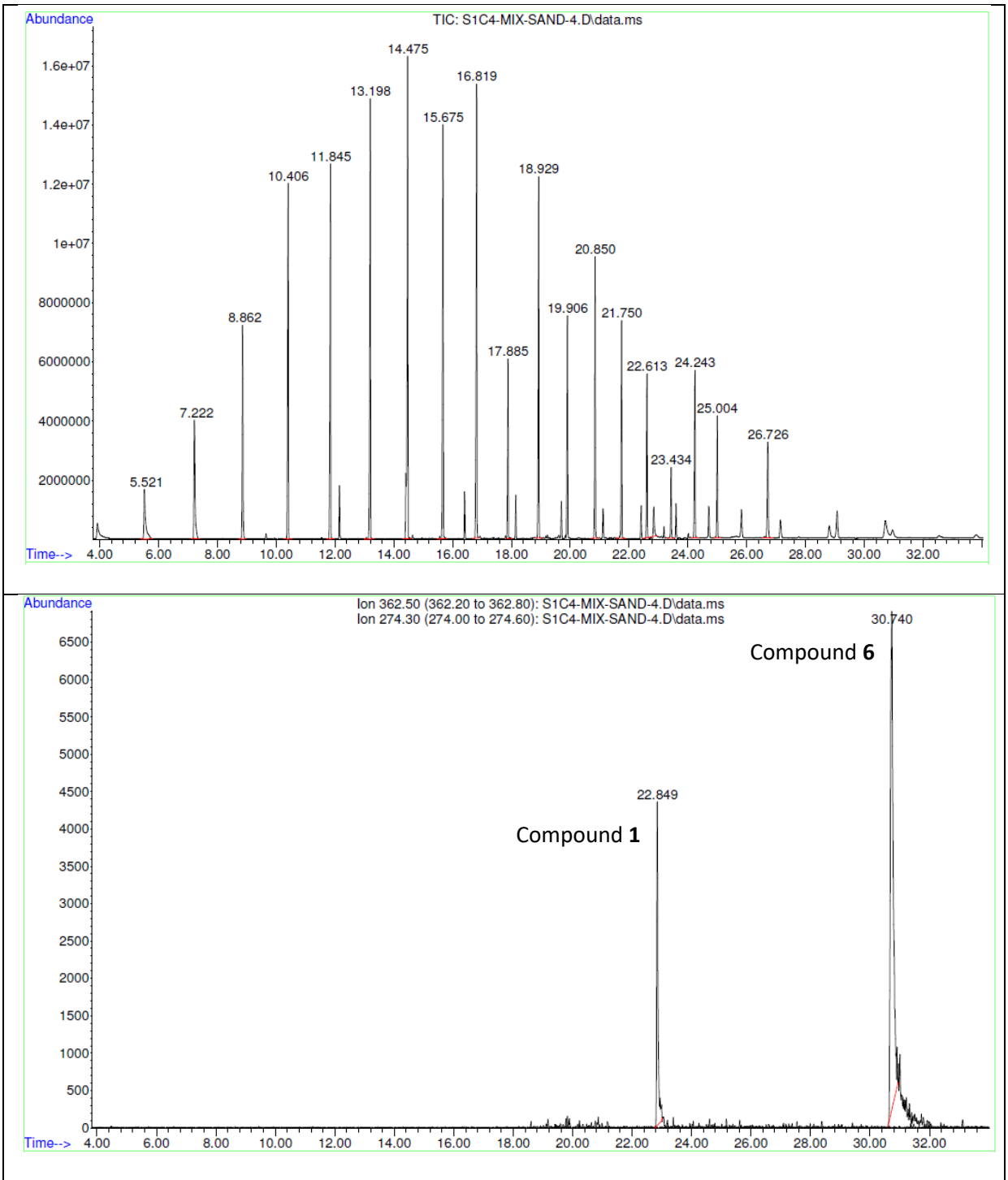

Figure S6. GC/EIMS total ion chromatogram of dichloromethane extract of soil spiked with compound **1** and **6** along with hydrocarbon mixture (top)
Bottom: GC/MS extracted ion chromatogram (*m/z* 274 and *m/z* 362) representing compound **1** and **6** (bottom).