

## Supporting Info

### Eco-friendly peelable active nanocomposite films designed for Biological and Chemical Warfare Agents decontamination

Gabriela Toader <sup>1, ‡</sup>, Aurel Diacon <sup>2, ‡</sup>, Traian Rotariu <sup>1,\*</sup>, Mioara Alexandru <sup>3,\*</sup>, Edina Rusen <sup>2</sup>, Raluca Elena Ginghină <sup>4</sup>, Florentina Alexe <sup>4</sup>, Ramona Oncioiu <sup>4</sup>, Florina Lucica Zorila <sup>3</sup>, Alice Podaru <sup>1</sup>, Andreea Elena Moldovan <sup>1</sup>, Daniela Pulpea <sup>1</sup>, Ana Mihaela Gavrila <sup>5</sup>, Tanta Verona Iordache <sup>5</sup> and Raluca Șomoghi <sup>5, 6</sup>

<sup>1</sup> Military Technical Academy “Ferdinand I”, 39-49 George Cosbuc Boulevard, 050141 Bucharest, Romania;

<sup>2</sup> Faculty of Applied Chemistry and Materials Science, University ‘Politehnica’ of Bucharest, 1-7 Gh. Polizu Street, 011061 Bucharest, Romania;

<sup>3</sup> Microbiology Laboratory of Horia Hulubei National Institute for R&D in Physics and Nuclear Engineering, 30 Reactorului St., 077125 Bucharest – Măgurele, Romania;

<sup>4</sup> Research and Innovation Center for CBRN Defense and Ecology, 225 Soseaua Oltenitei, 041327 Bucharest, Romania;

<sup>5</sup> National Institute of Research and Development for Chemistry and Petrochemistry, 202 Splaiul Independentei, 060041 Bucharest, Romania;

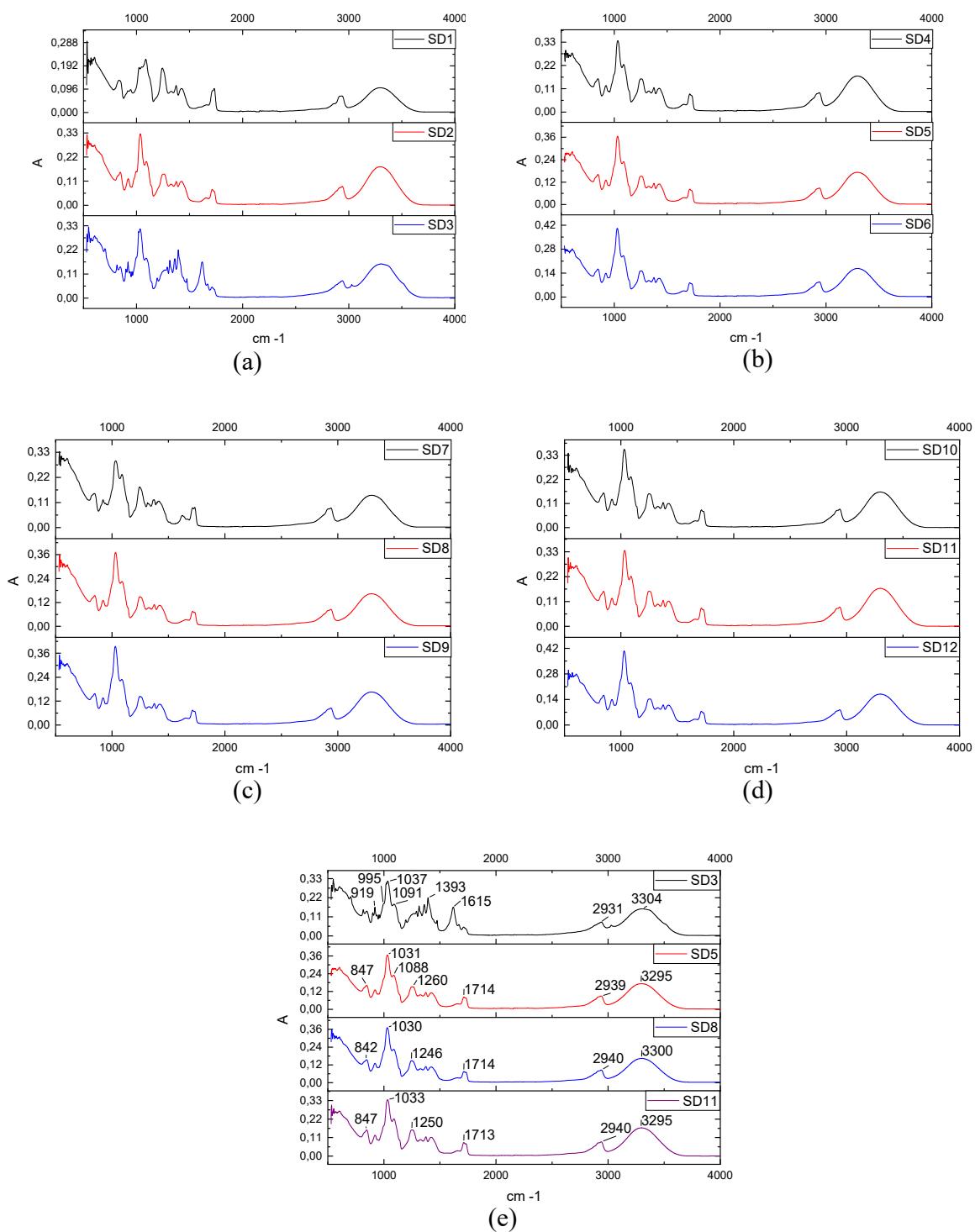
<sup>6</sup> Petroleum-Gas University of Ploiesti, 100680 Ploiesti, Romania

\*Correspondence: traian.rotariu@mta.ro (T.R.), mioara.alexandru@nipne.ro (M.A.)

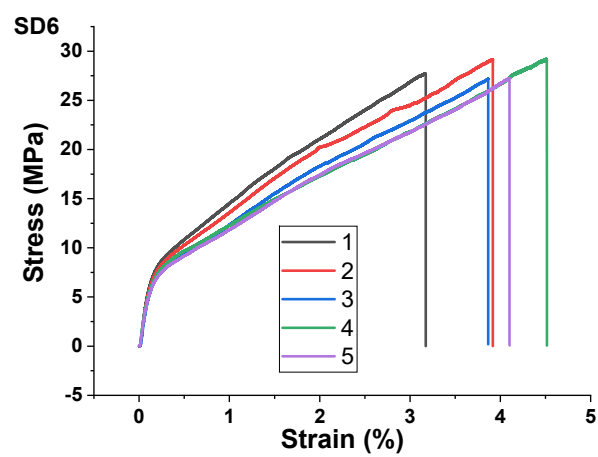
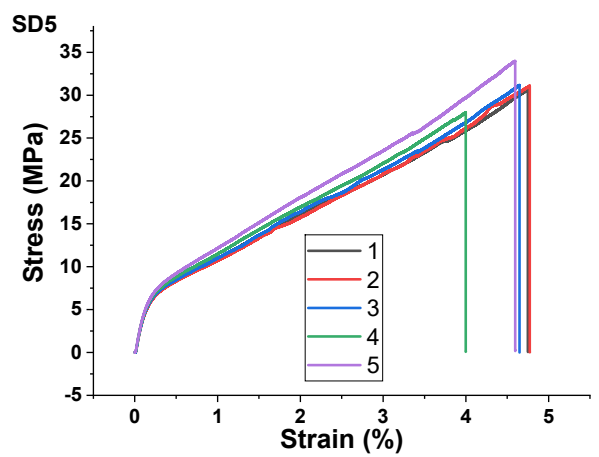
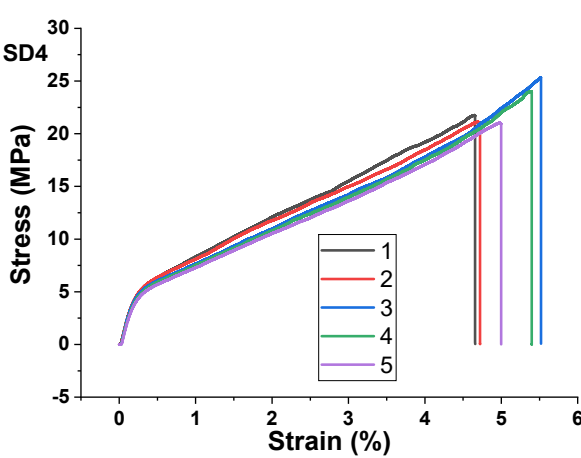
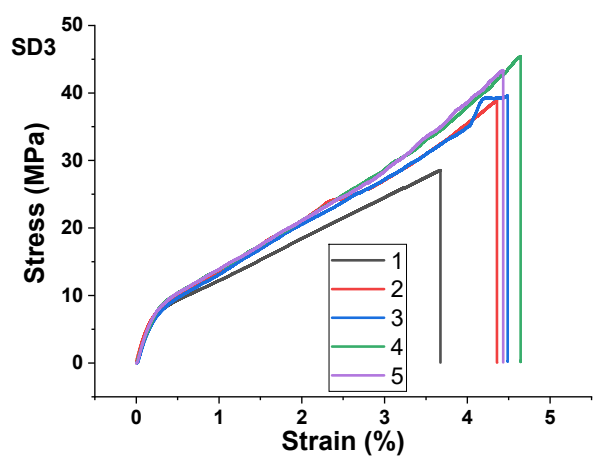
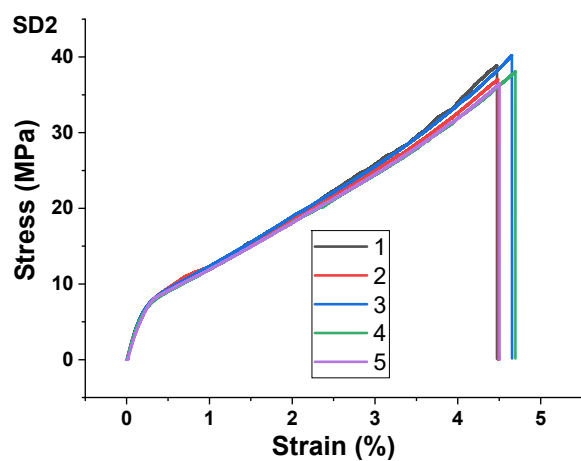
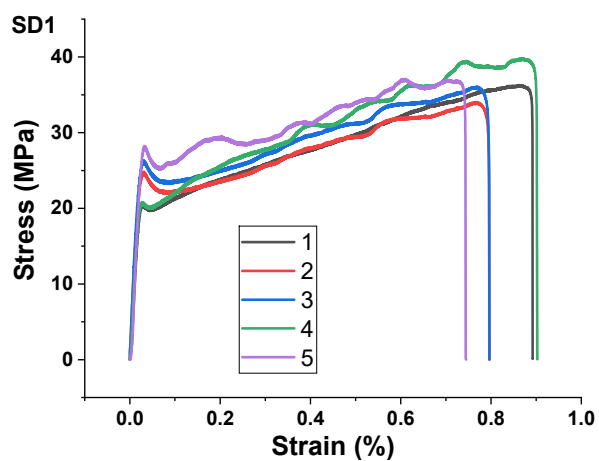
‡ Co-first authors, equally contributed to this study

**Table S1.** *Evaporation rate of the decontamination solutions*

Sample	Evaporation rate (%wt./h)			
	25 °C	30 °C	35 °C	40 °C
SD1	5.5	10.2	15.4	23.0
SD2	5.5	10.1	15.6	21.4
SD3	5.5	9.6	13.1	22.5
SD4	4.9	8.6	14.4	20.6
SD5	5.5	8.5	14.7	21.5
SD6	5.4	9.8	15.2	21.8
SD7	5.3	10.4	15.9	23.3
SD8	6.0	11.4	16.9	23.3
SD9	6.1	10.4	15.6	21.9
SD10	6.2	10.6	16.5	22.2
SD11	5.0	10.0	16.0	23.7
SD12	5.6	10.2	16.1	23.6



**Figure S1.** FT-IR spectra of the polymer nanocomposite films.



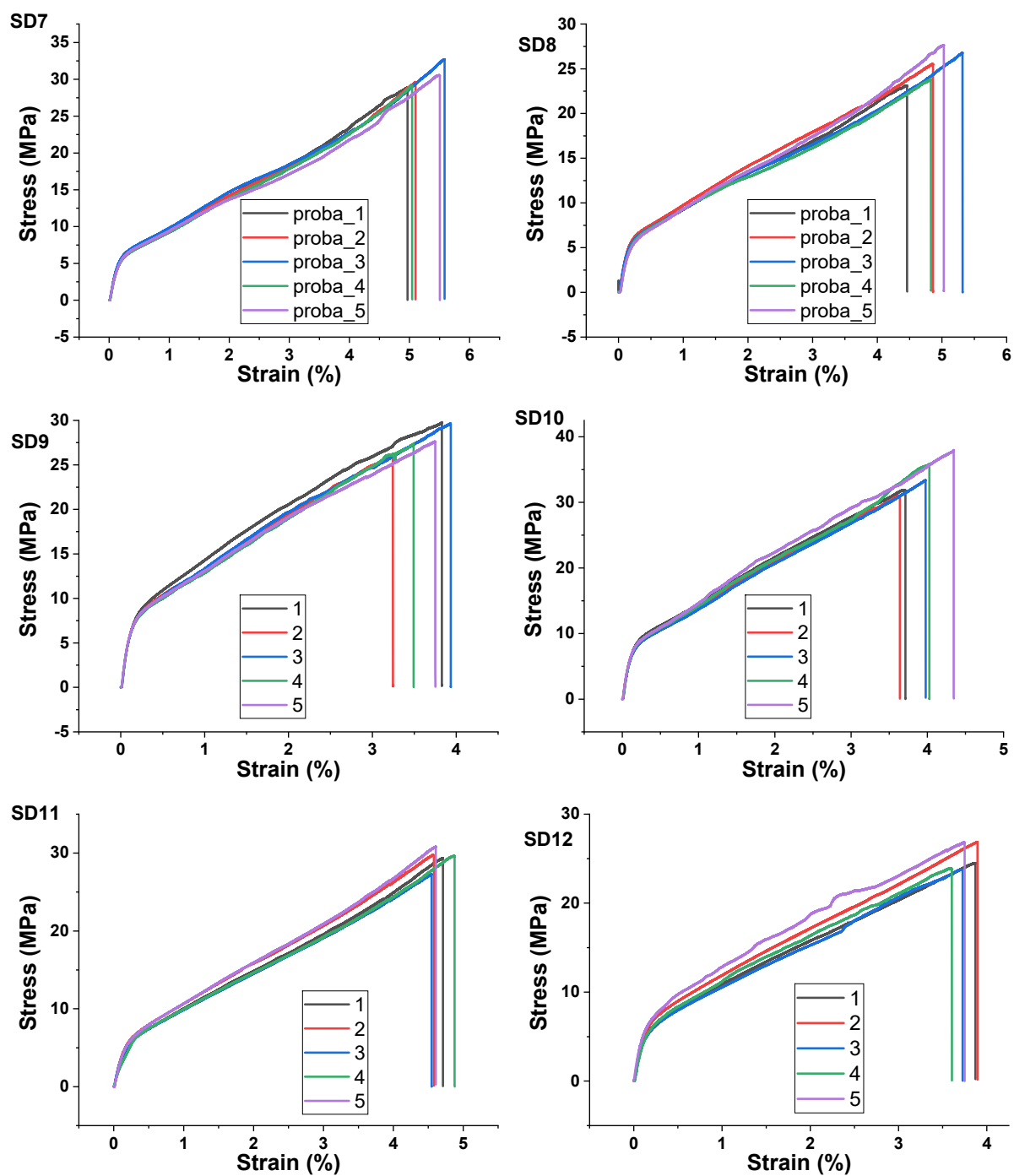
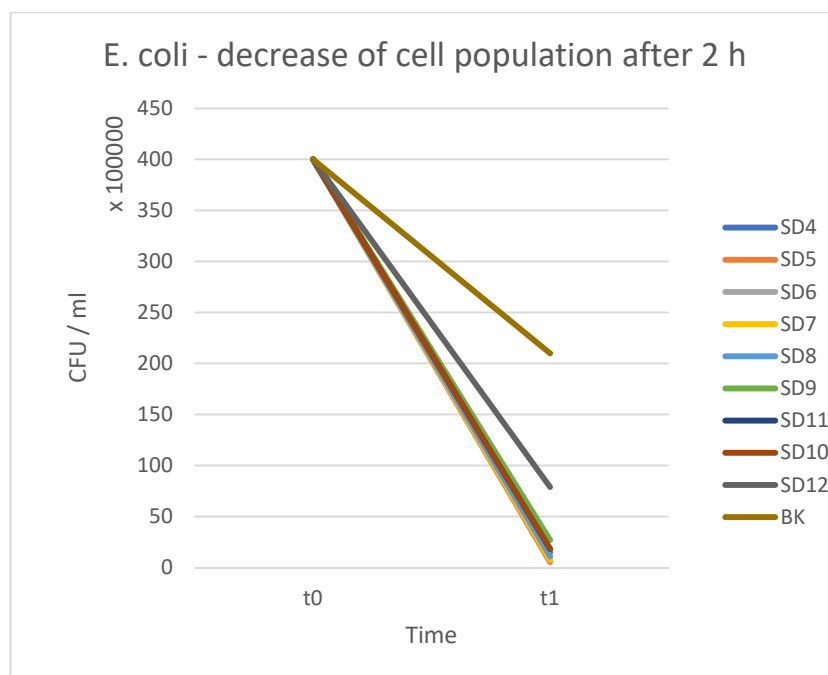


Figure S2. Tensile tests results.

**Table S2.** Tensile tests results.

Sample	$\epsilon_{\max}$ (%)	$\sigma_{\max}$ (MPa)	Young modulus (MPa)
SD1	0.8769	36.0593	41.123
SD2	4.6537	40.1990	8.638
SD3	4.4317	43.3565	9.783
SD4	4.9943	20.9684	4.198
SD5	4.5949	33.9905	7.397
SD6	4.0999	27.2418	6.644
SD7	5.0431	29.1408	5.778
SD8	4.8274	23.8357	4.938
SD9	3.7492	27.6316	7.370
SD10	4.6081	30.8314	6.691
SD11	3.9761	33.3954	8.399
SD12	3.8693	24.5156	6.336

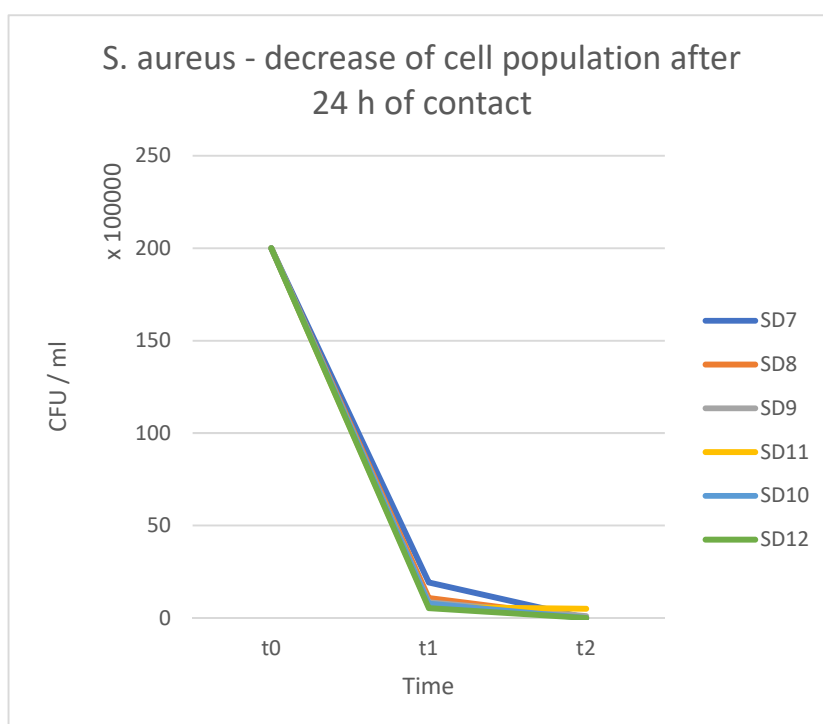
### Biological decontamination tests



**Figure S3.** Cell population after 2 hours in contact with the decontamination solutions for *E. coli*.

**Table S3.** Antimicrobial activity of the decontamination solutions against *E.coli*.

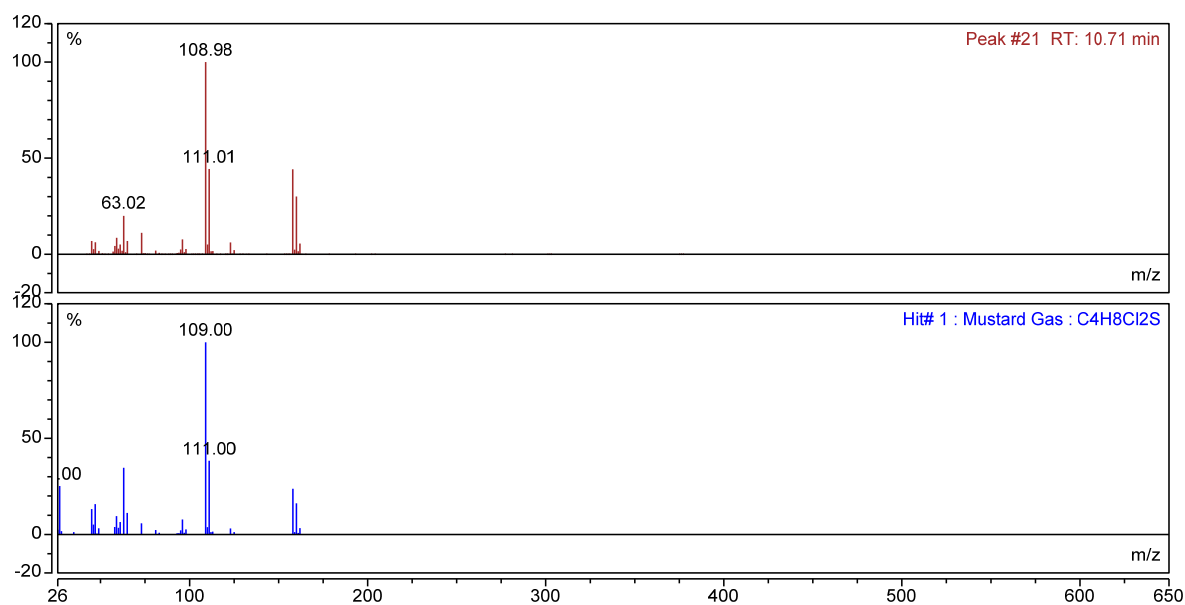
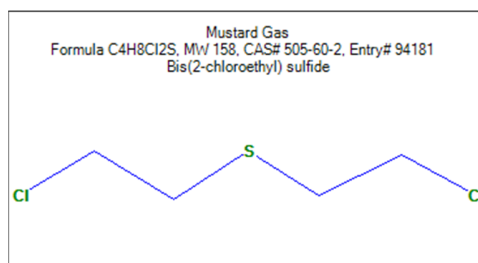
	SD4 (UFC / mL)	SD5 (UFC / mL)	SD6 (UFC / mL)	SD7 (UFC / mL)	SD8 (UFC / mL)	SD9 (UFC / mL)	SD10 (UFC / mL)	SD11 (UFC / mL)	SD12 (UFC / mL)	SD3 (UFC / mL)
<b>T<sub>0</sub></b> (10 <sup>5</sup> UFC / ml)	52 × 10 <sup>5</sup>	65 × 10 <sup>5</sup>	50 × 10 <sup>5</sup>	45 × 10 <sup>5</sup>	65 × 10 <sup>5</sup>	200 × 10 <sup>5</sup>	59 × 10 <sup>5</sup>	53 × 10 <sup>5</sup>	49 × 10 <sup>5</sup>	280 × 10 <sup>5</sup>
<b>T<sub>1</sub></b> (10 <sup>5</sup> UFC / mL)	4.5 × 10 <sup>5</sup>	5.1 × 10 <sup>5</sup>	3.8 × 10 <sup>5</sup>	8.9 × 10 <sup>5</sup>	50 × 10 <sup>5</sup>	100 × 10 <sup>5</sup>	43 × 10 <sup>3</sup>	35 × 10 <sup>3</sup>	25 × 10 <sup>3</sup>	250 × 10 <sup>5</sup>

**Figure S4.** Cell population after 24 hours in contact with the decontamination solutions for *E. coli*.**Table S4.** Antimicrobial activity of the decontamination solutions against *S. aureus*.

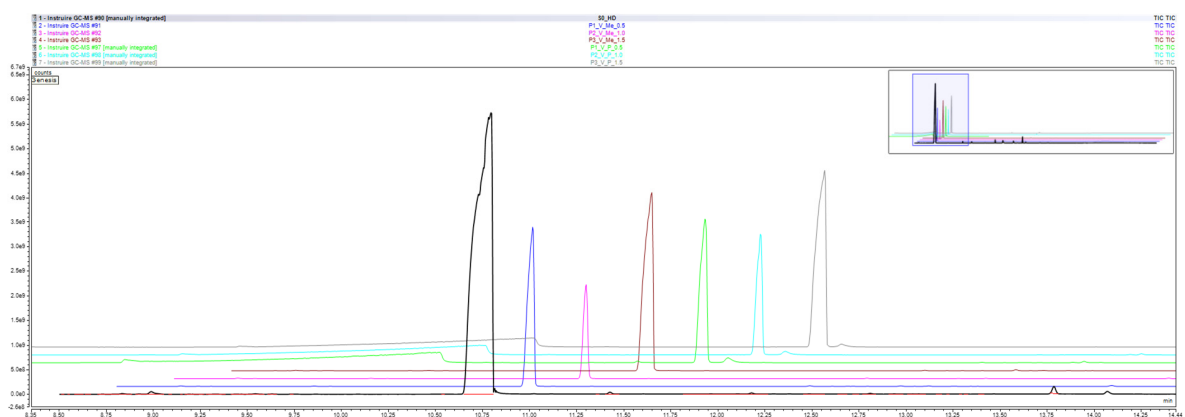
	SD4 (UFC / mL)	SD5 (UFC / mL)	SD6 (UFC / mL)	SD7 (UFC / mL)	SD8 (UFC / mL)	SD9 (UFC / mL)	SD10 (UFC / mL)	SD11 (UFC / mL)	SD12 (UFC / mL)	SD3 (UFC / mL)
<b>T<sub>0</sub></b> (10 <sup>5</sup> UFC / mL)	320 × 10 <sup>5</sup>	290 × 10 <sup>5</sup>	90 × 10 <sup>5</sup>	40 × 10 <sup>5</sup>	32 × 10 <sup>5</sup>	290 × 10 <sup>5</sup>	250 × 10 <sup>5</sup>	270 × 10 <sup>5</sup>	290 × 10 <sup>5</sup>	300 × 10 <sup>5</sup>
<b>T<sub>1</sub></b> (10 <sup>5</sup> UFC / mL)	289 × 10 <sup>5</sup>	66 × 10 <sup>5</sup>	43 × 10 <sup>5</sup>	< 10 <sup>2</sup>	< 10 <sup>2</sup>	10 <sup>3</sup>	2 × 10 <sup>3</sup>	< 10 <sup>2</sup>	< 10 <sup>2</sup>	290 × 10 <sup>5</sup>

## Chemical Decontamination tests

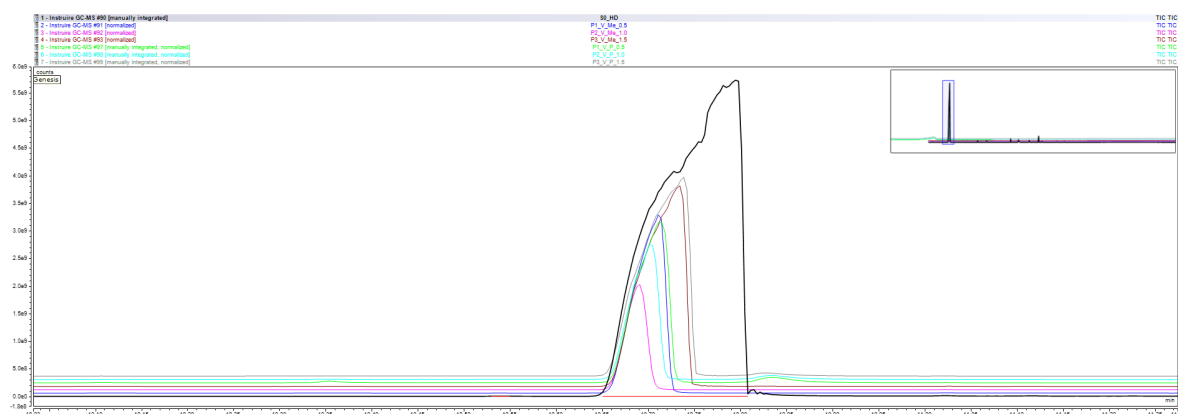
### Sulphur mustard



**Figure S5.** Mass spectra of HD (up – from analysis; down – NIST database), RT – 10.71 min.

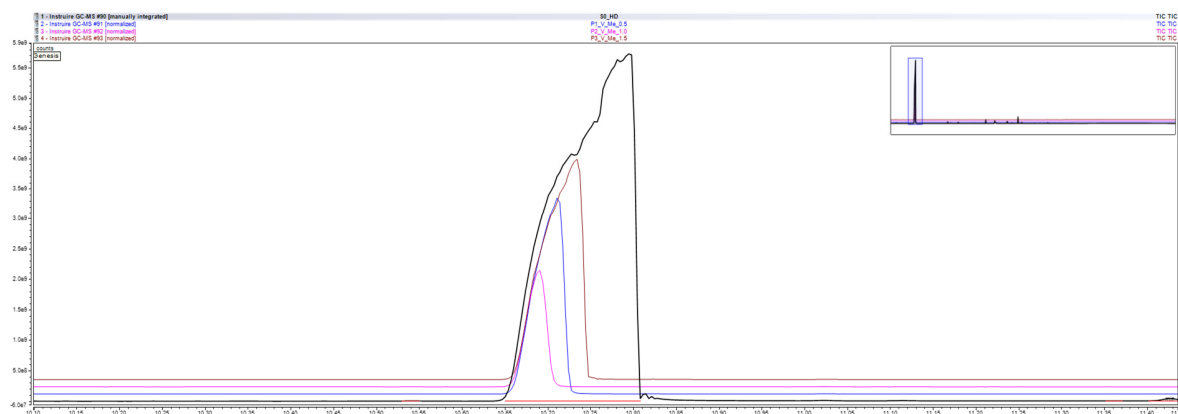


**Figure S6.** Chromatograms multigraph.



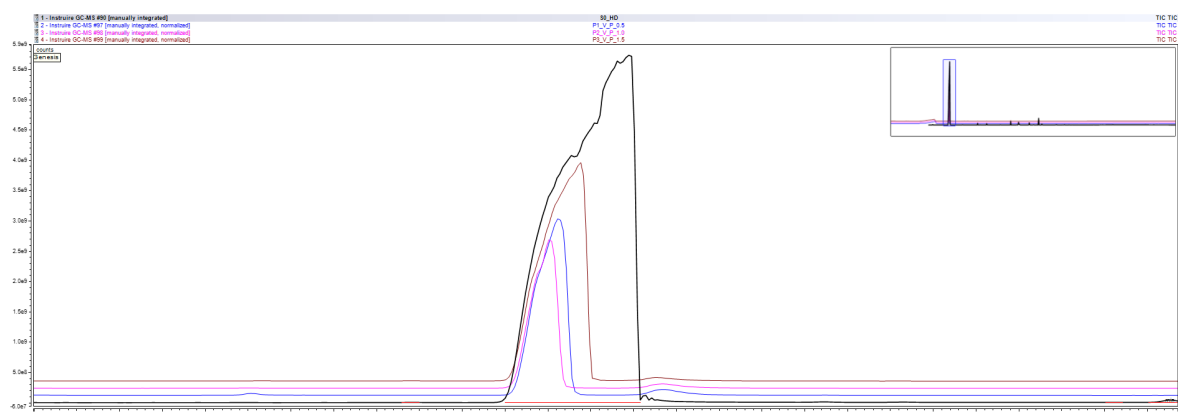
**Figure S7.** Total Ions Chromatograms overlap for all samples, representing HD at the RT (retention time): 10.70;

(blank - initial HD contamination; blue - residual HD after decontamination with SD10, extracted with DCM from the metallic surface; magenta - residual HD after decontamination with SD11, extracted with DCM from the metallic surface; burgundy - residual HD after decontamination with SD12, extracted with DCM from the metallic surface; green – unreacted HD found after decontamination in peeled film SD10, extracted with DCM; cyan - unreacted HD found after decontamination in peeled film SD11, extracted with DCM; gray - unreacted HD found after decontamination in peeled film SD12, extracted with DCM).



**Figure S8.** Chromatograms overlap for reference sample and samples extracted from the metallic surface after decontamination.

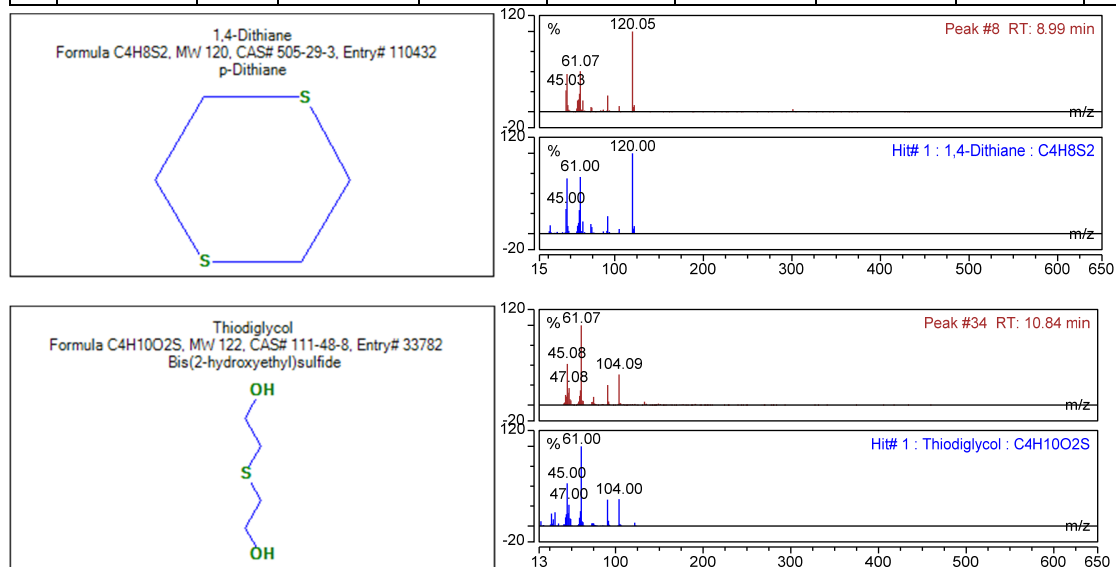


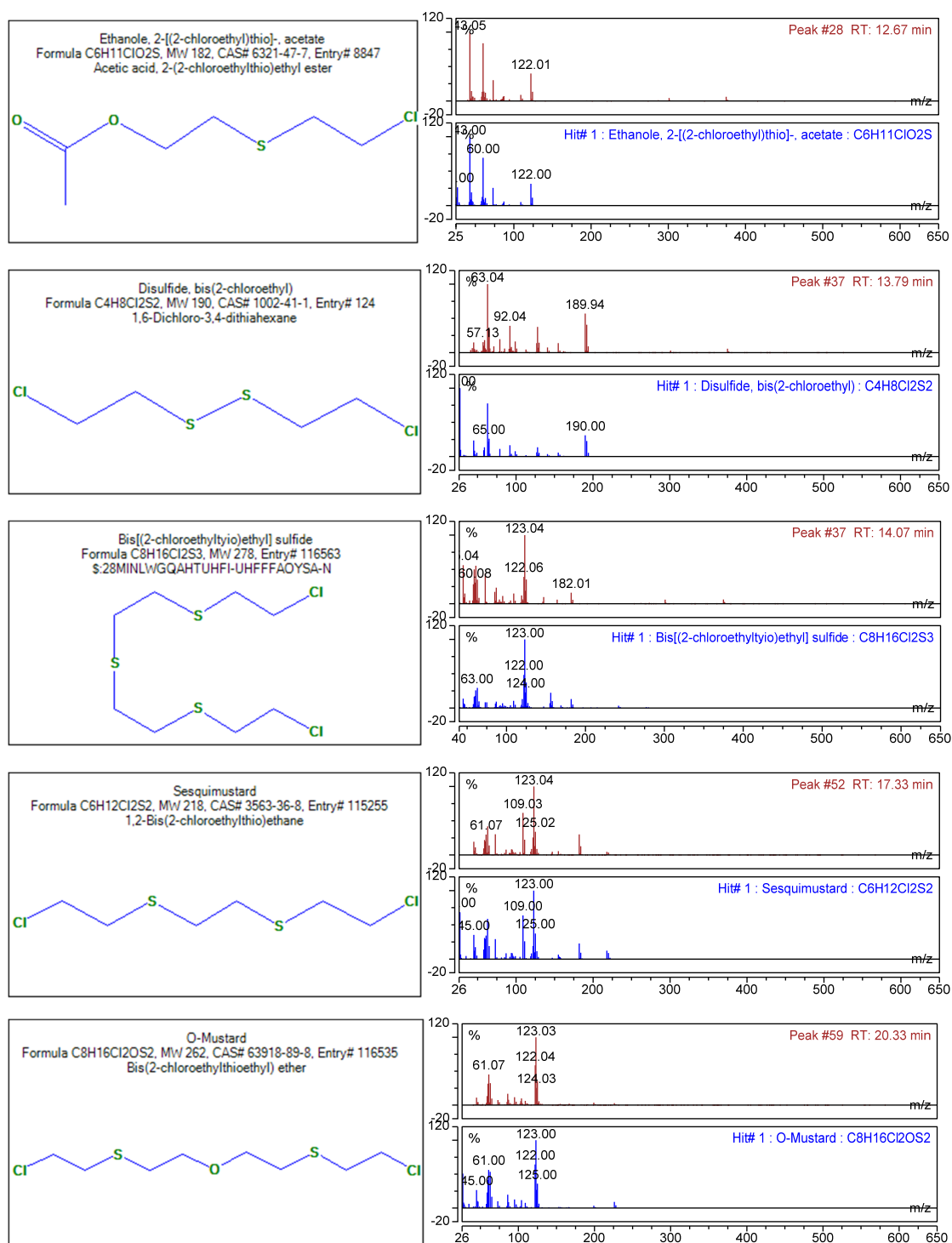


**Figure S9.** Chromatograms overlap for reference sample and samples extracted from the nanocomposite film after decontamination.

**Table S5.** Degradation products of HD monitored during the decontamination process.

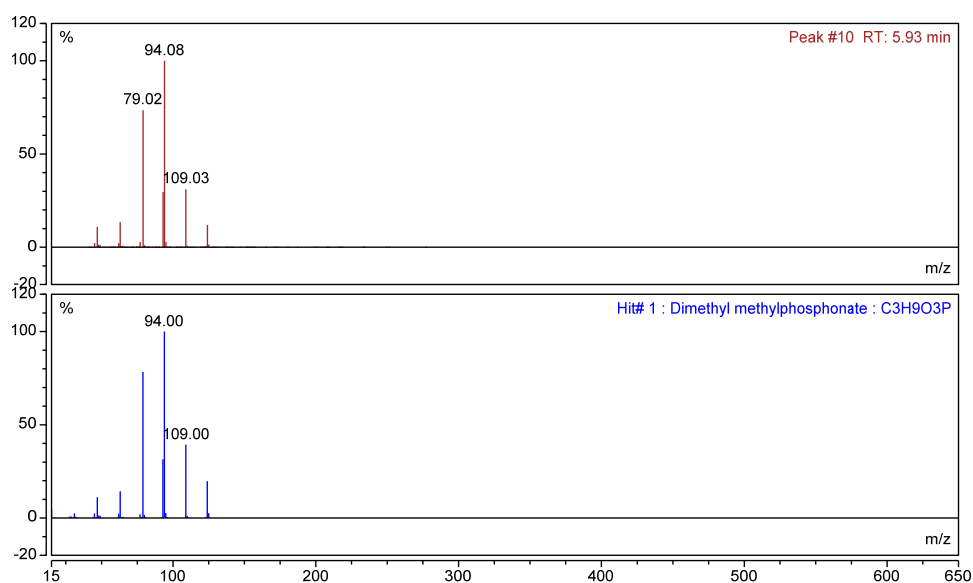
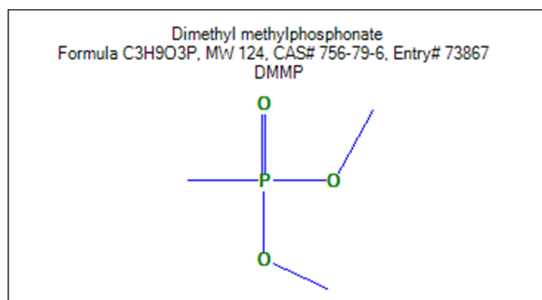
No	Compound	RT	AS0	AP1Me	AP2Me	AP3Me	AP1P	AP2P	AP3P
1	Dithiane	8.99	1887741	124343	32416	114606	0	0	0
2	HD	10.79	568555828	12350046 1	51799820	189174524	119498537	82888058	207352784
3	Thiodiglycol (TDG)	10.84	0	0	0	0	4218280	3269076	2301103
4	Etanol 2-((2-chloroethyl)thio) 1-acetate	12.67	0	268287	129480	515104	200100	190421	563526
5	Bis(2-chloroethyl) disulfide	13.78	3485028	475053	252378	547932	378536	194092	453803
6	Bis((2-chloroethylthio)ethyl)sulfide	14.07	1270521	0	0	0	0	0	0
7	Sesqui-mustard	17.33	7045057	662471	208319	895429	782569	978155	1386415
8	O-mustard	20.33	14223291	1097079	314214	1449068	1172060	2040661	2238374



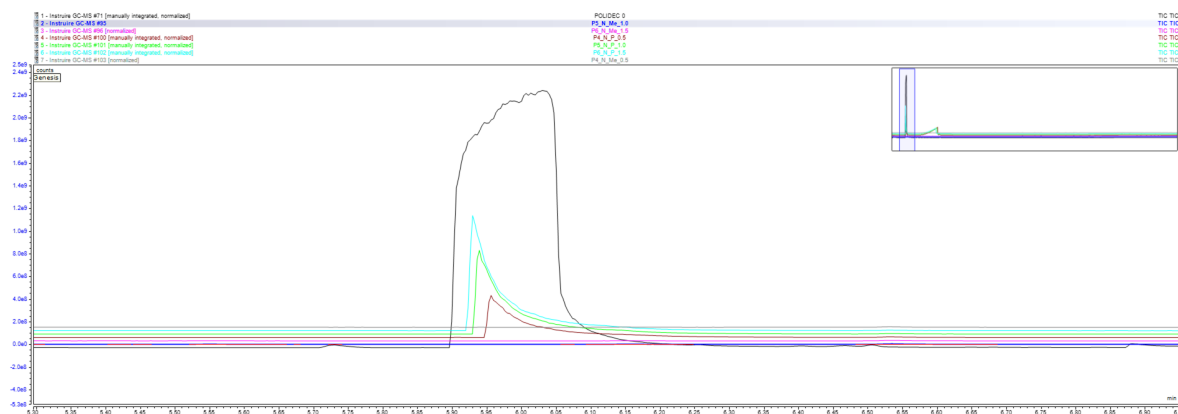


**Figure S10.** Degradation products of Yperite.

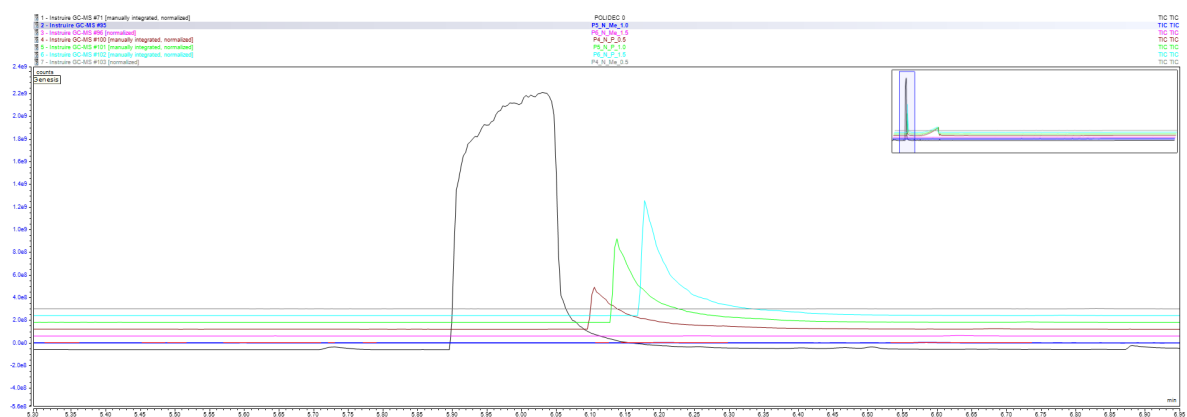
## Dimethyl methylphosphonate



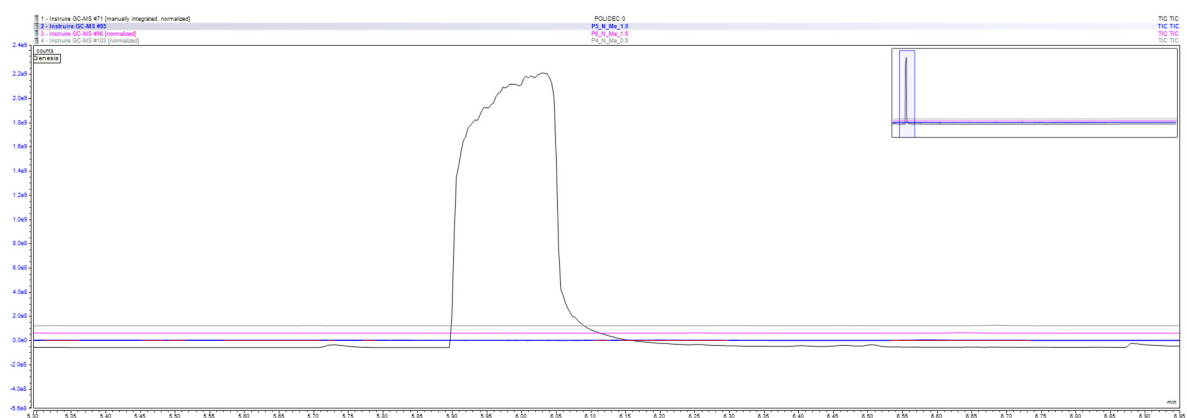
**Figure S11.** Mass spectra of HD (up – from analysis; down – NIST database) RT – 5.93 min.



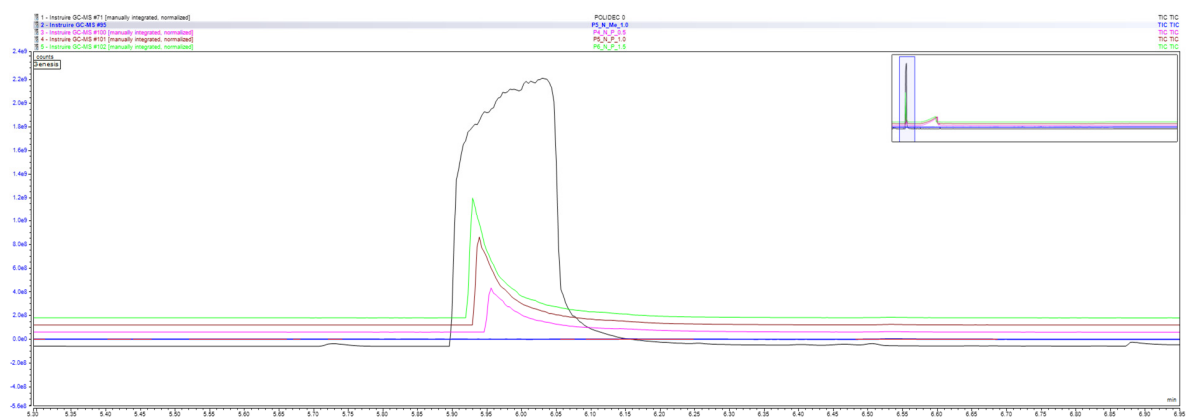
**Figure S12.** Chromatograms overlap for all samples.



**Figure S13.** Chromatograms overlap for all samples.



**Figure S14.** Chromatograms overlap for reference sample and samples extracted from the metallic surface after decontamination.



**Figure S15.** Chromatograms overlap for reference sample and samples extracted from the nanocomposite film after decontamination.