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Chemical regeneration of granular activated carbon: preliminary evaluation of alternative regenerant solutions

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Supplementary Information

1. Desorption kinetics

The maximum desorption efficiency using each regenerant solution was achieved within 120 mins, which is a range of time required in performing chemical regeneration[18].

1.1. High purity Reverse Osmosis (RO) water

The desorption efficiency of the target contaminants using high purity RO water at room temperature was almost negligible.

1.2. Sodium hydroxide (NaOH)

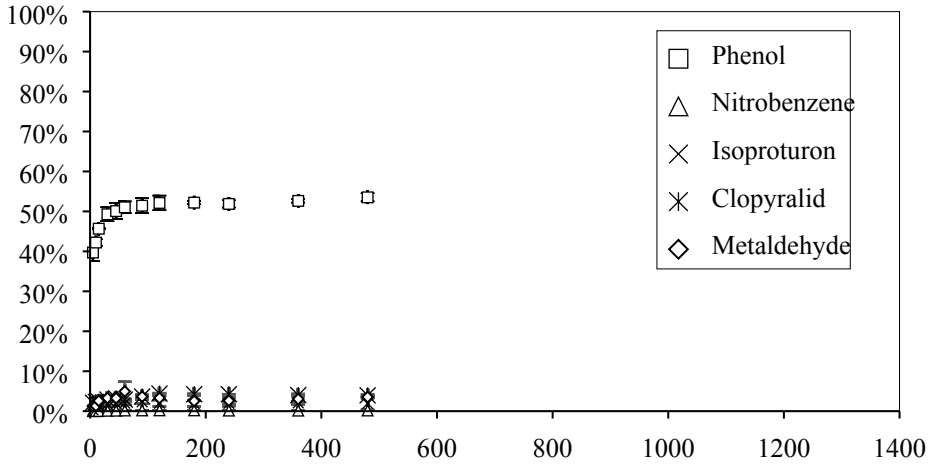


Figure S1. Desorption kinetics (DE –vs- time) of the target contaminants using sodium hydroxide.

1.3. Ethanol (CH_3CH_2OH)

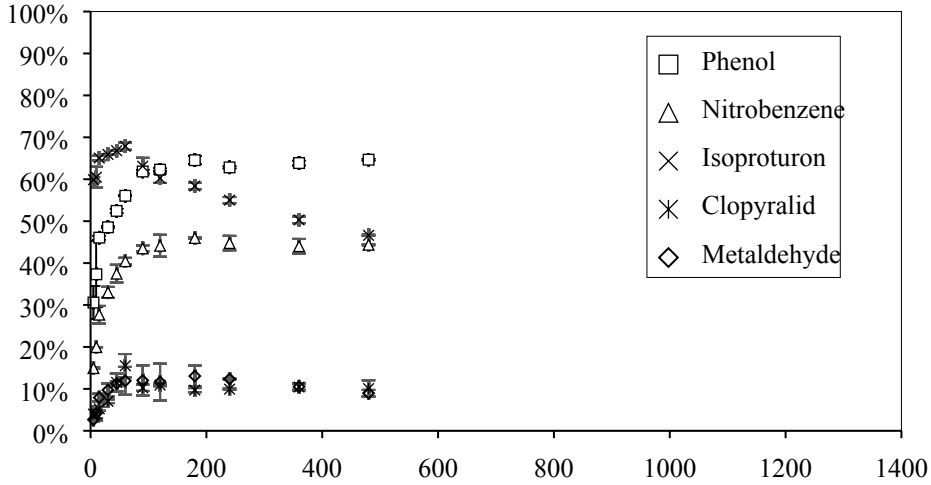


Figure S2. Desorption kinetics (DE –vs- time) of the target contaminants using ethanol.

1.4. A mixture of sodium hydroxide and ethanol ($NaOH/CH_3CH_2OH$)

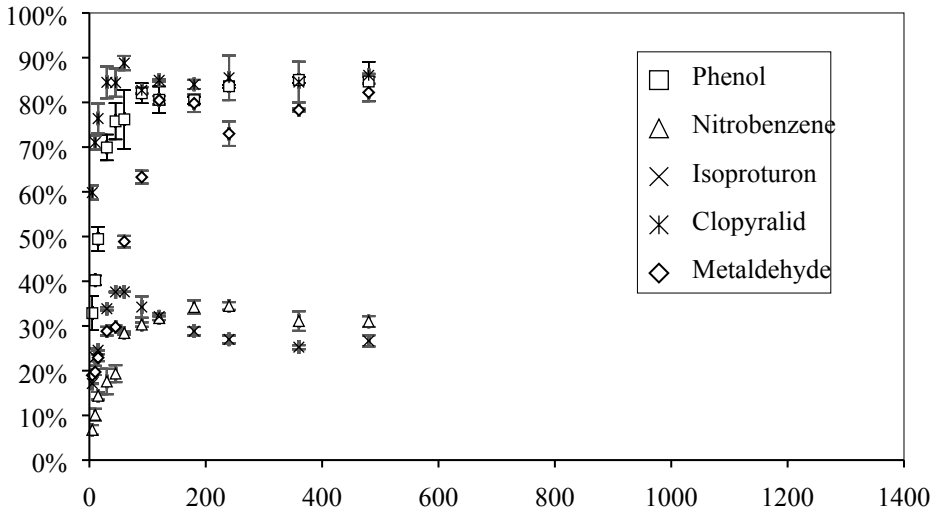
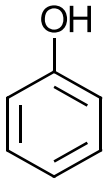
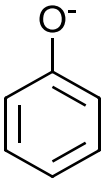
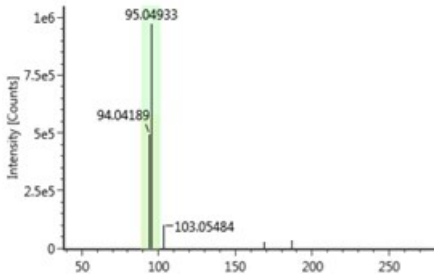
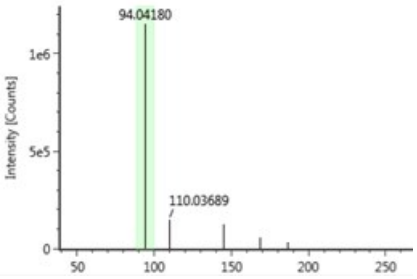
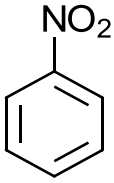
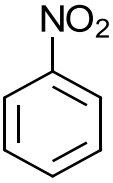
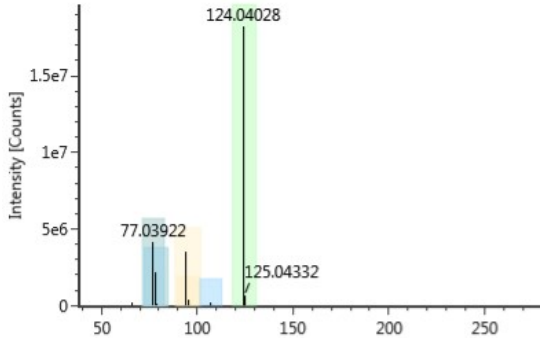
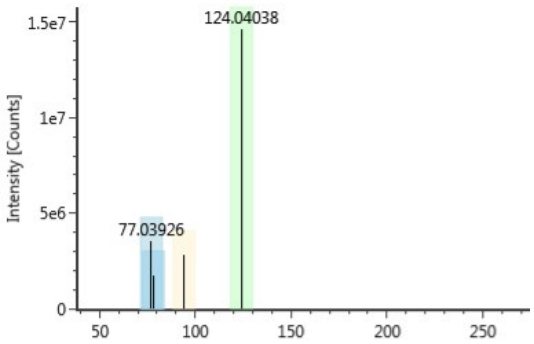
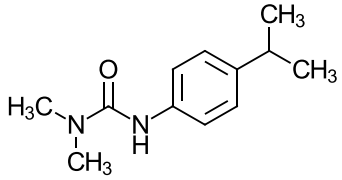
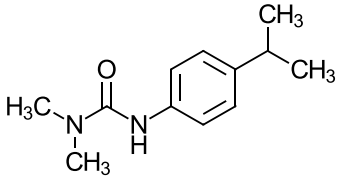


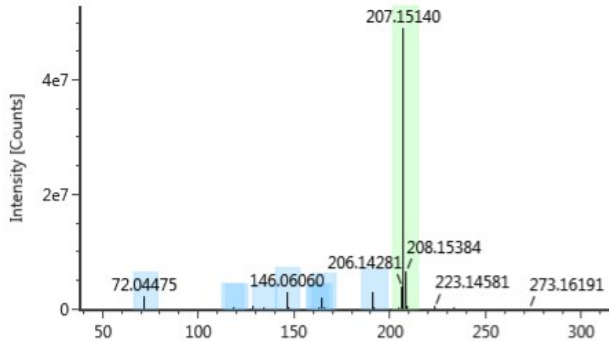
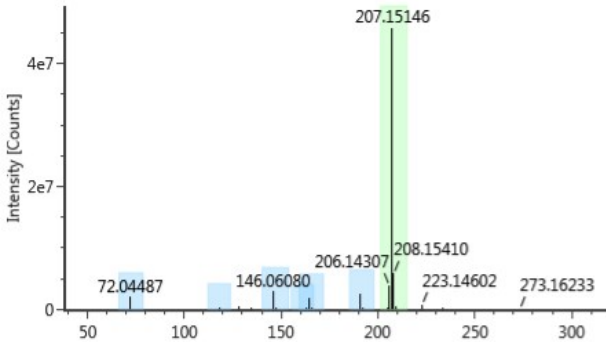
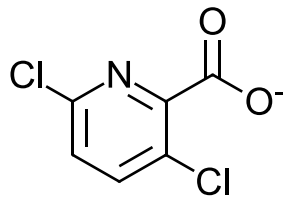
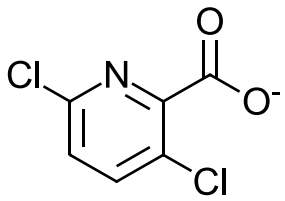
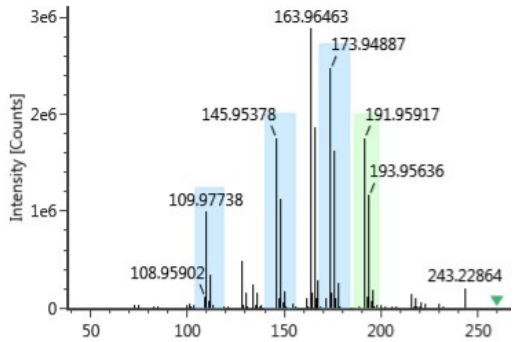
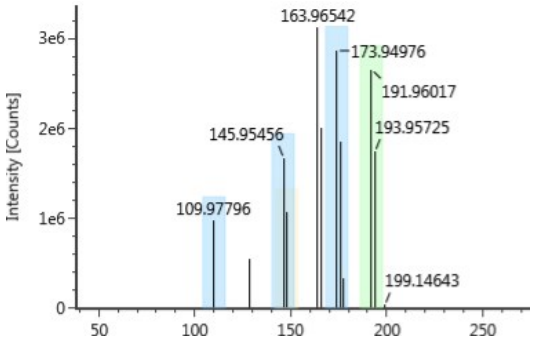
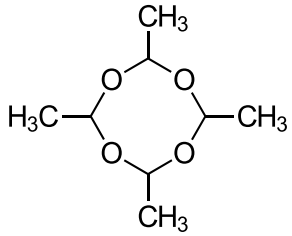
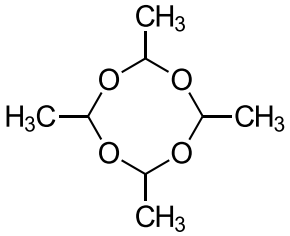
Figure S3. Desorption kinetics (DE –vs- time) of the target contaminants using a mixture of NaOH/ CH_3CH_2OH.

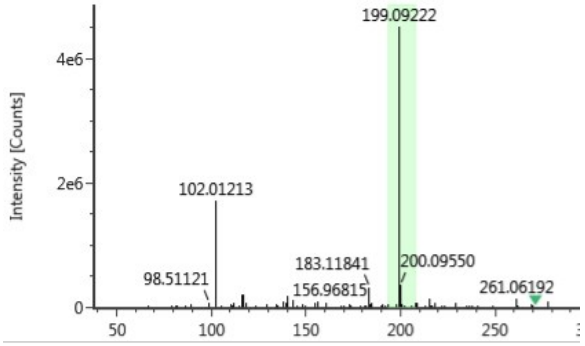
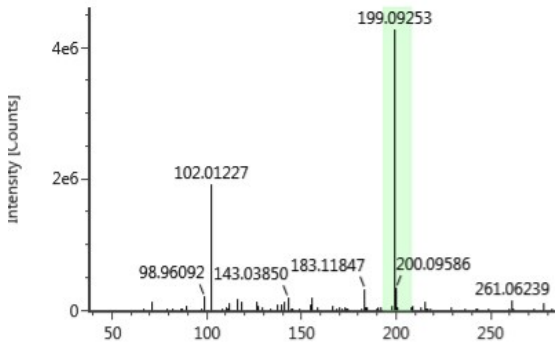
2. Mass spectra

The mass spectra of the target contaminants upon the exposure of the $NaOH/CH_3CH_2OH$ mixture at low energy conditions are shown in **Table S1**.

44 **Table S1.** Mass spectra of the target contaminants in the $NaOH/CH_3CH_2OH$ mixture.

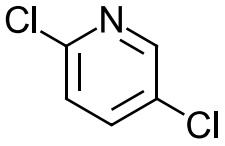
Most abundant form in H_2O at pH 7	**Proposed reaction product in $NaOH/CH_3CH_2OH$ at pH > 13**
Phenol	Phenolate
	
$[M + H^+] = 95$ m/z	$[M\text{-}H + H^+] = 94$ m/z
	
Nitrobenzene	Nitrobenzene
	
$[M + H^+] = 124$ m/z	$[M + H^+] = 124$ m/z
	
Isoproturon	Isoproturon
	
$[M + H^+] = 207$ m/z	$[M + H^+] = 207$ m/z

Most abundant form in H_2O at pH 7	Proposed reaction product in $NaOH/CH_3CH_2OH$ at pH > 13
	
Clopyralid	Clopyralid*
	
$[M\text{-}H + H^+]$ = 191.9 m/z	$[M\text{-}H + H^+]$ = 191.9 m/z
	
Metaldehyde	Metaldehyde
	
$[M + Na^+]$ = 199 m/z	$[M + Na^+]$ = 199 m/z

Most abundant form in H_2O at pH 7	Proposed reaction product in $NaOH/CH_3CH_2OH$ at pH > 13
	

Notes: Spectra with green shades were parent compound and the spectra in blue shades are fragments at low energy.

*Another potential form of clopyralid [M-H + H^+] = 147 m/z



This structure was likely to be formed only when clopyralid and the regenerant solution are mixed and then exposed at a high temperature (150 ^oC). If clopyralid was mixed with the regenerant solution at room temperature and its pH was adjusted at pH 7, the parent form of clopyralid was observed. This means that the regenerant solution did not change the structure or degrade clopyralid at room temperature (the same temperature that the desorption tests were conducted using the $NaOH/CH_3CH_2OH$ mixture).