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Detection of Oxygenated Aromatics in Atmospheric Anisole Flames

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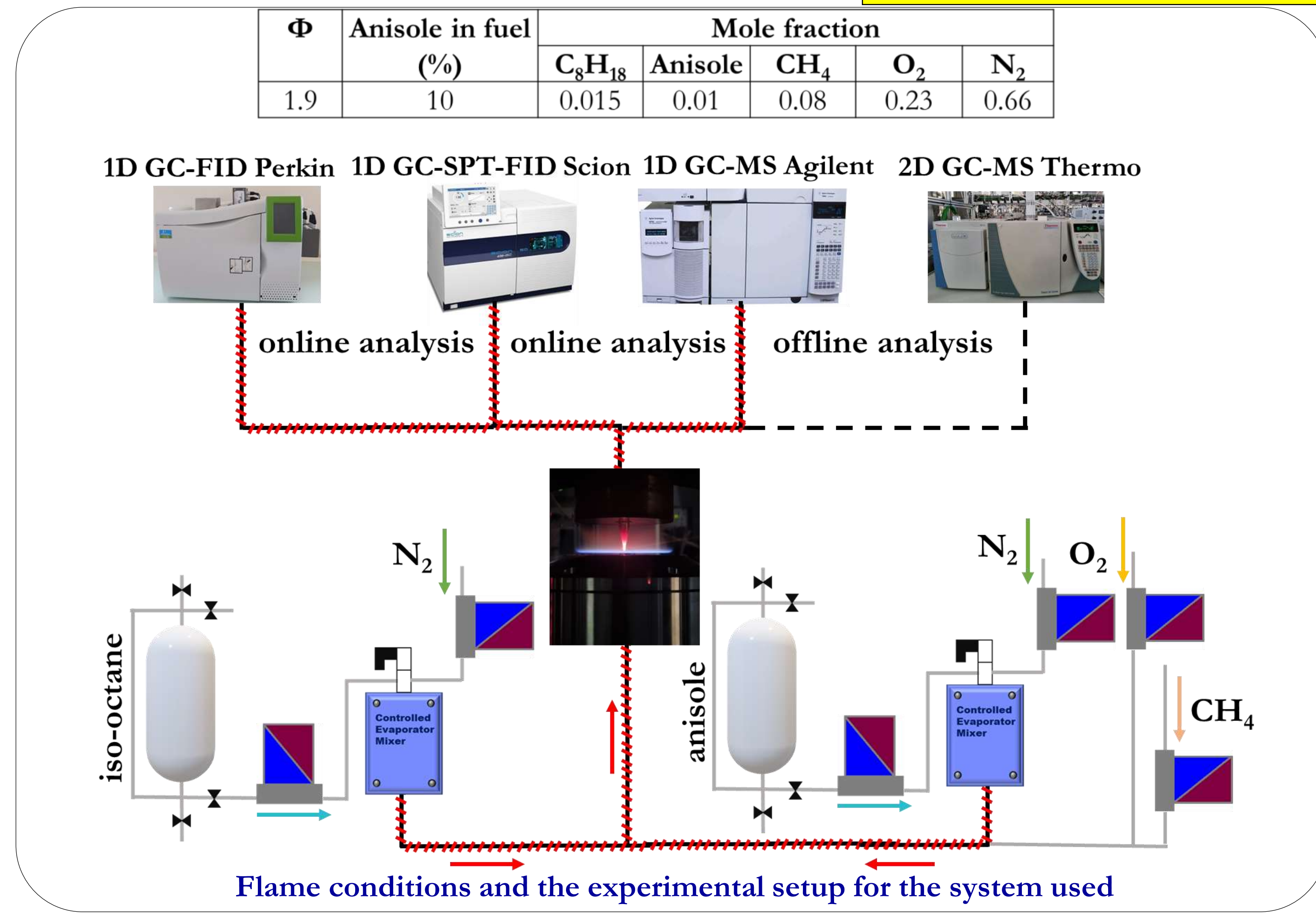
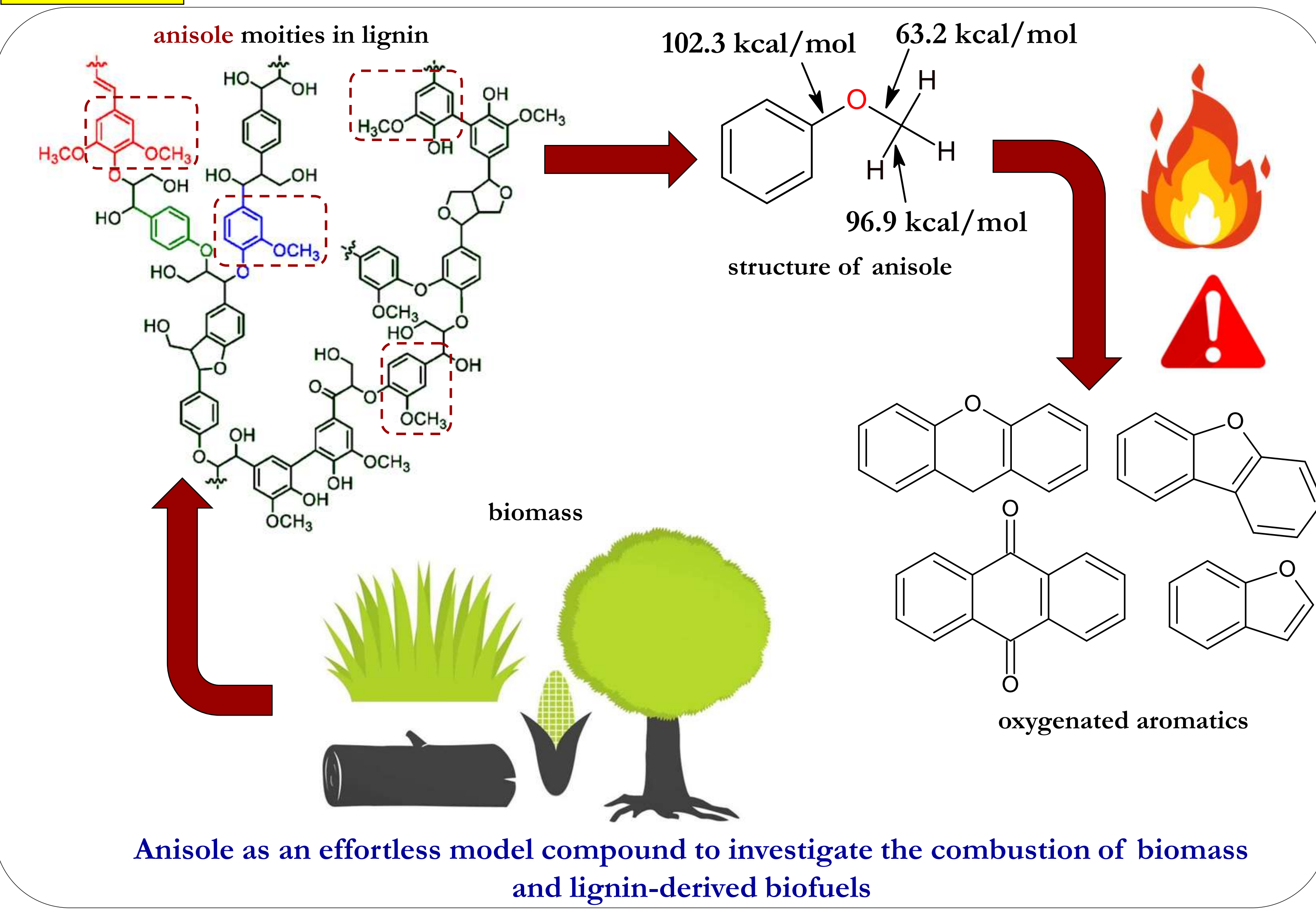
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Context

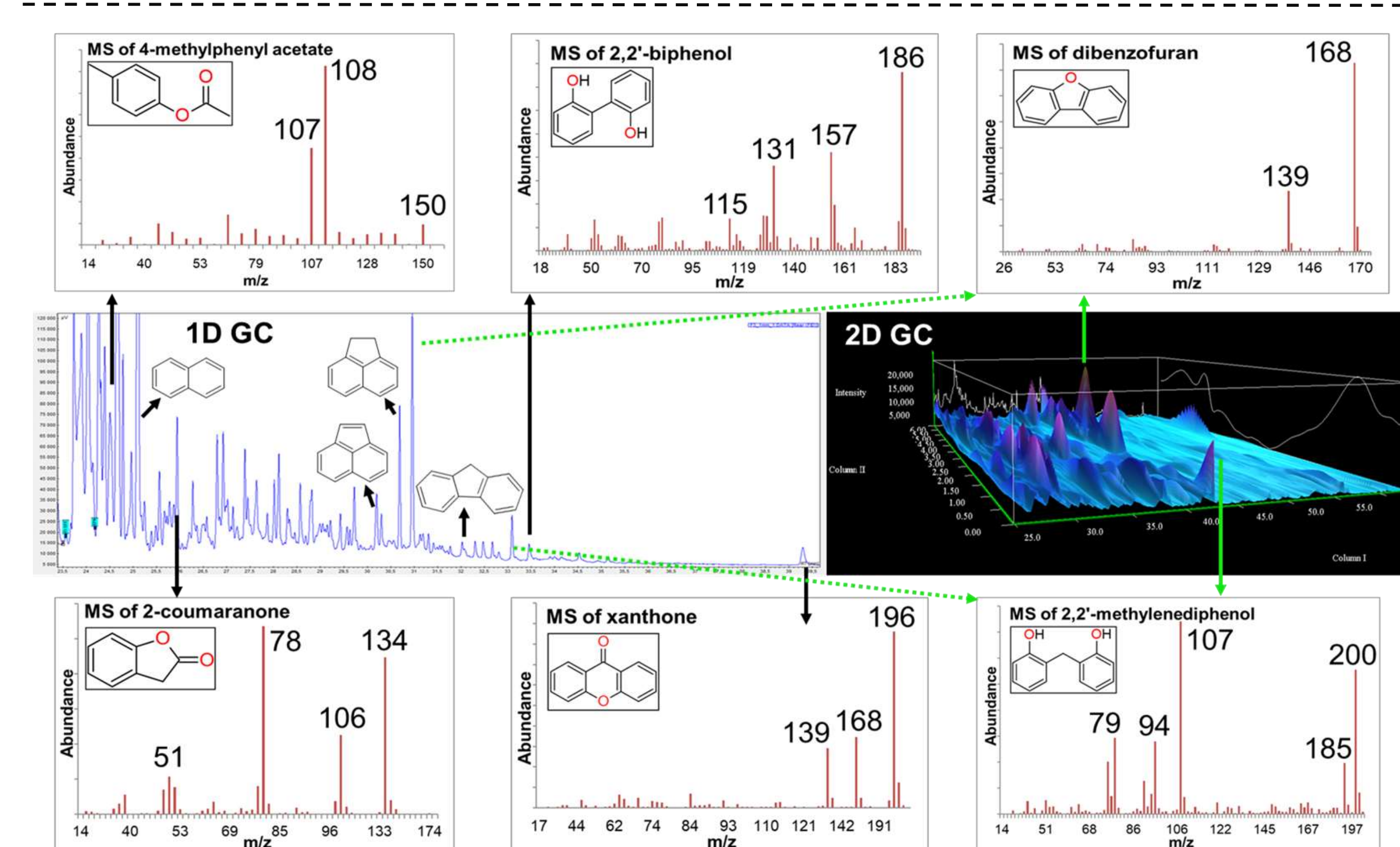
Experimental method



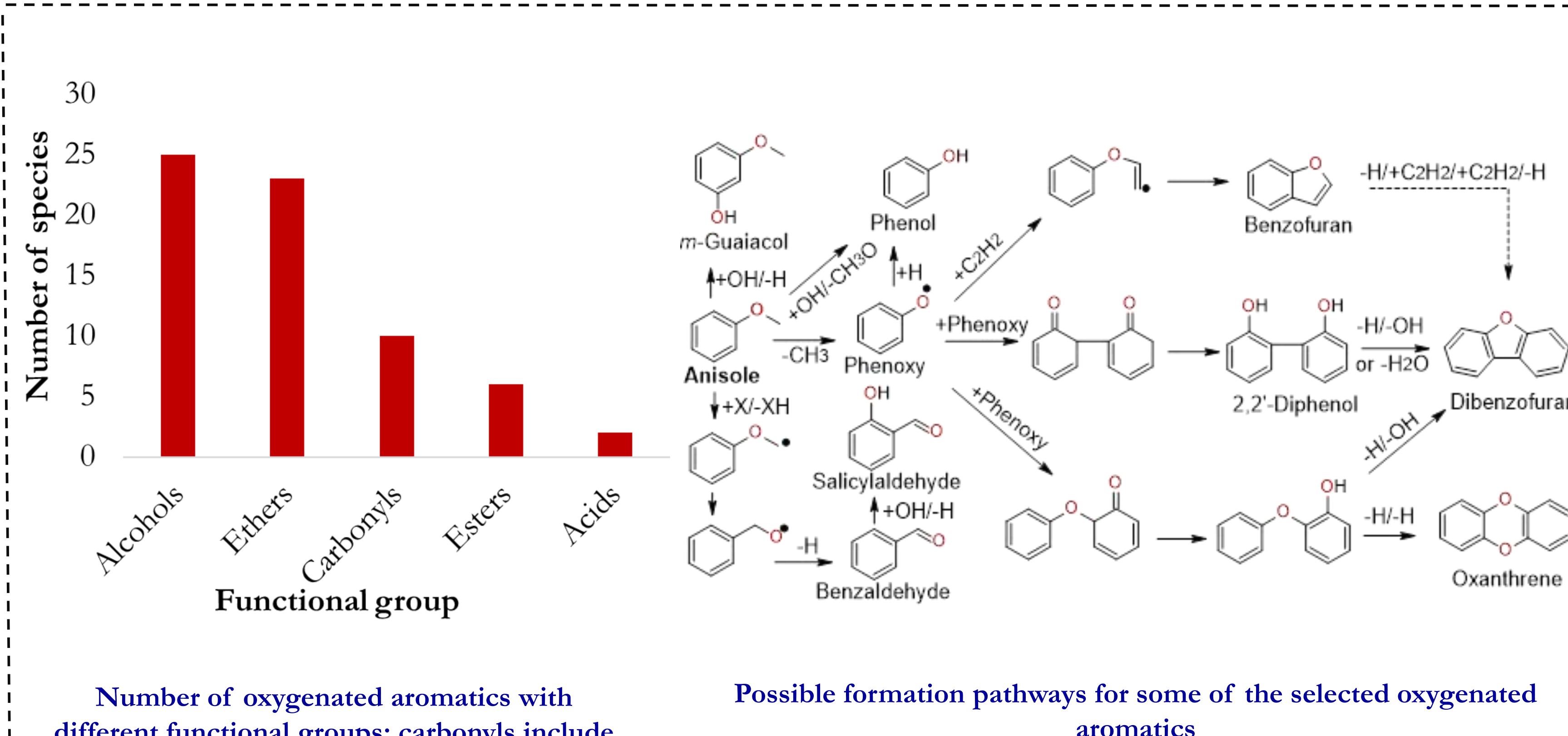
Results

M	Formula	Name	Structure
94	C ₆ H ₆ O	Phenol	
106	C ₇ H ₆ O	Benzaldehyde	
108	C ₇ H ₈ O	Anisole	
	C ₇ H ₈ O	<i>o</i> -Cresol; 2-Methylphenol	
	C ₇ H ₈ O	<i>m</i> -Cresol; 3-Methylphenol	
	C ₇ H ₈ O	<i>p</i> -Cresol; 4-Methylphenol	
110	C ₆ H ₆ O ₂	Hydroquinone; Benzene-1,4-diol	
118	C ₈ H ₆ O	Benzofuran; 1-Benzofuran	
120	C ₈ H ₈ O	Dihydrobenzofuran; 2,3-Dihydro-1-benzofuran	
122	C ₇ H ₆ O ₂	Salicylaldehyde; 2-Hydroxybenzaldehyde	
	C ₇ H ₆ O ₂	<i>m</i> -Formylphenol; 3-Hydroxybenzaldehyde	
	C ₇ H ₆ O ₂	1,3-Benzodioxole; 2H-1,3-benzodioxole	
	C ₈ H ₁₀ O	Ethyl phenyl ether; Ethoxybenzene	
	C ₈ H ₁₀ O	2,6-Xylenol; 2,6-Dimethylphenol	
	C ₈ H ₁₀ O	2-Ethyl phenol	
124	C ₇ H ₈ O ₂	<i>m</i> -Guaiaicol; 3-Methoxyphenol	
132	C ₉ H ₈ O	1-Indanone; 2,3-Dihydro-1H-inden-1-one	
	C ₉ H ₈ O	Cinnamaldehyde; (2E)-3-Phenylprop-2-enal	
134	C ₈ H ₆ O ₂	2-Coumaranone; 1-Benzofuran-2(3H)-one	
136	C ₈ H ₈ O ₂	<i>p</i> -Toluic acid; 4-Methylbenzoic acid	
	C ₉ H ₁₂ O	5-Ethyl <i>m</i> -cresol; 3-Ethyl-5-methylphenol	
144	C ₁₀ H ₈ O	2-Vinyl benzofuran; 2-Ethynyl-1-benzofuran	
	C ₁₀ H ₈ O	1-Naphthol; Naphthalen-1-ol	
146	C ₁₀ H ₁₀ O	1-Methylindan-2-one; 1-Methyl-1,3-dihydro-2H-inden-2-one	
	C ₁₀ H ₁₀ O	2-Ethyl benzofuran; 2-Ethyl-1-benzofuran	
150	C ₉ H ₁₀ O ₂	<i>o</i> -Acetoxy toluene; 2-Methylphenyl acetate	
	C ₉ H ₁₀ O ₂	<i>p</i> -Acetoxy toluene; 4-Methylphenyl acetate	
156	C ₁₁ H ₈ O	Phenyl propionate; Phenyl propanoate	
162	C ₁₁ H ₁₄ O	2-Naphthaldehyde; Naphthalen-2-carbaldehyde	
168	C ₁₂ H ₈ O	2,2-dimethyl-3,4-dihydro-2H-1-Benzopyran	
170	C ₁₂ H ₁₀ O	Diphenyl ether; 1,1'-Oxydibenzene	
	C ₁₂ H ₁₀ O	Hydroxybiphenyl; [1,1'-Biphenyl]-2-ol	
	C ₁₂ H ₁₀ O	1-Naphthyl vinyl ether; 1-(Ethenyloxy)naphthalene	
180	C ₁₃ H ₈ O	9-Fluorenone; 9H-Fluoren-9-one	
182	C ₁₃ H ₁₀ O	Xanthene; 9H-Xanthene	
	C ₁₃ H ₁₀ O	9-Fluorenyl; 9H-Fluoren-9-yl	
	C ₁₃ H ₁₀ O	4-Methylidibenzofuran	
	C ₁₃ H ₁₀ O	6H-Dibenzo[<i>b,d</i>]pyran	
184	C ₁₂ H ₈ O ₂	Dibenzo- <i>p</i> -dioxin; Oxanthrene	
	C ₁₂ H ₈ O ₂	2-Dibenzofuranol; Dibenzo[<i>b,d</i>]furan-2-ol	
	C ₁₃ H ₁₂ O	Benzyl phenyl ether; (Benzoyloxy)benzene	
	C ₁₃ H ₁₂ O	<i>o</i> -Benzylphenol; 2-Benzylphenol	
	C ₁₃ H ₁₂ O	<i>p</i> -Benzylphenol; 4-Benzylphenol	
186	C ₁₂ H ₁₀ O ₂	Diphenyl ether; [1,1'-Biphenyl]-2,2'-diol	
	C ₁₂ H ₁₀ O ₂	<i>m</i> -Phenoxy phenol; 3-Phenoxyphenol	
	C ₁₂ H ₁₀ O ₂	1-Naphthyl acetate; Naphthalen-1-yl acetate	
	C ₁₃ H ₁₄ O	2-((2-Naphthyl)-2-propanol); 2-(Naphthalen-2-yl)propan-2-ol	
	C ₁₃ H ₁₄ O	2,5,8-Trimethylnaphthalen-1-ol	
196	C ₁₃ H ₈ O ₂	Xanthone; 9H-Xanthene-9-one	
198	C ₁₄ H ₁₄ O	1,2,3,4-tetrahydrophenanthren-4-ol	
200	C ₁₃ H ₁₂ O ₂	Bis(2-hydroxyphenyl) methane; 2,2'-Methylenediphenol	
	C ₁₃ H ₁₂ O ₂	2-((4-Hydroxyphenyl)methyl)phenol	
208	C ₁₄ H ₈ O ₂	Anthraquinone; Anthracene-9,10-dione	
212	C ₁₃ H ₁₆ O	1,1-Diphenyl-1-methoxyethane; 1,1'-(1-Methoxyethane-1,1-diyloxy)dibenzene	
224	C ₁₃ H ₁₂ O ₂	9-Fluorenyl acetate; 9H-Fluoren-9-yl acetate	
226	C ₁₄ H ₁₀ O ₃	Xanthene-9-carboxylic acid; 9H-Xanthene-9-carboxylic acid	

Identified oxygenated aromatics; M represents the molar mass of the species in g/mol



Examples of chromatograms (middle panel) obtained in the doped anisole flame at 1.5 mm above the burner surface; some mass spectra GC-MS are also presented



Number of oxygenated aromatics with different functional groups; carbonyls include aldehydes and ketones.

Possible formation pathways for some of the selected oxygenated aromatics

Conclusions and Perspectives

- >60 oxygenated aromatics have been identified in an anisole doped using advanced Gas Chromatography
- More than half of these oxygenates amongst these have been reported for the first time
- Quantification of these aromatic oxygenates is currently an ongoing step
- Simulations will be performed allowing a precise interpretation of the effects of the oxygenated additives
- Other than the gas phase investigation, experiments to probe the particulates in the flames have also been envisioned.

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