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# Detection of Oxygenated Aromatics in Atmospheric Anisole Flames

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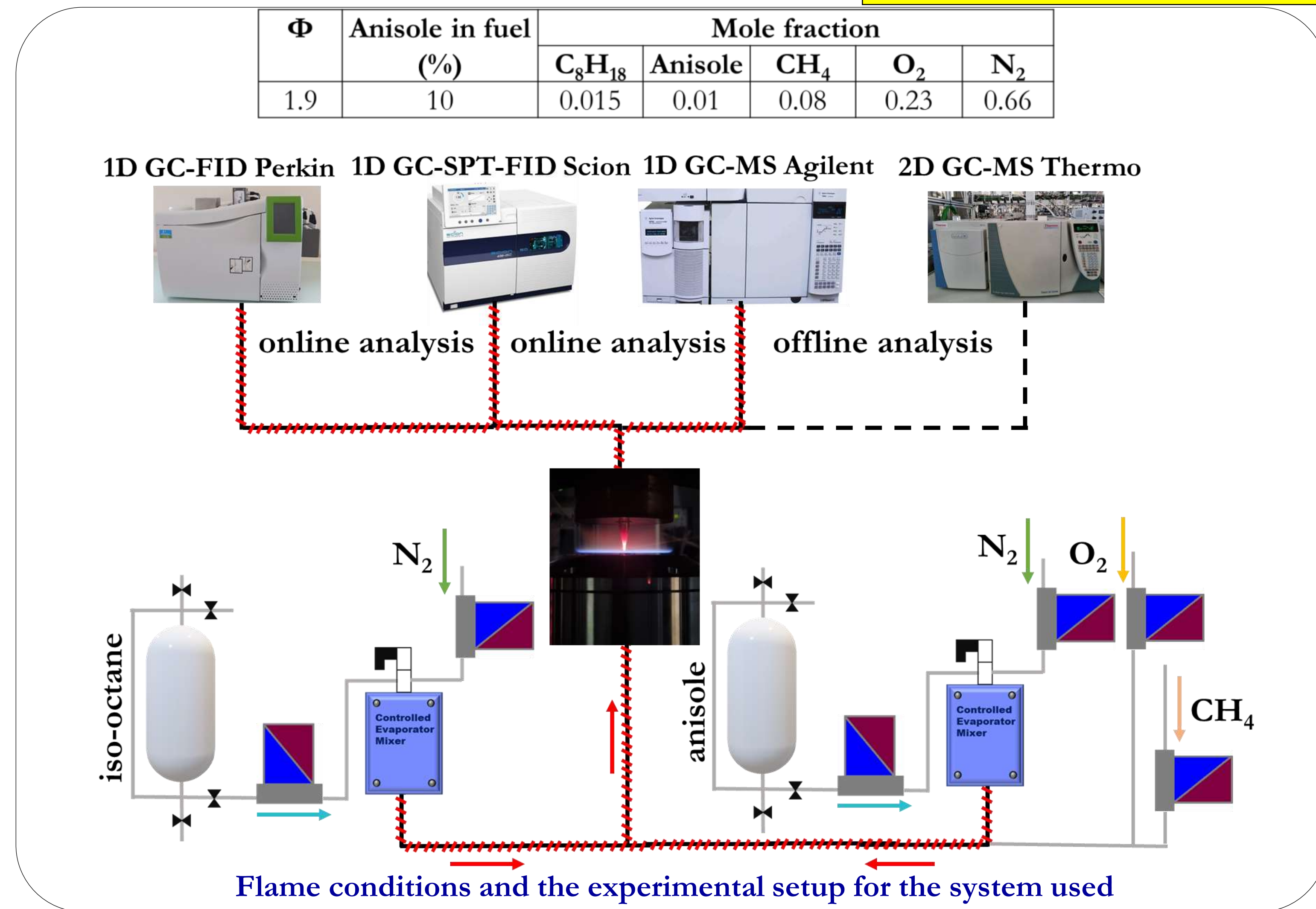
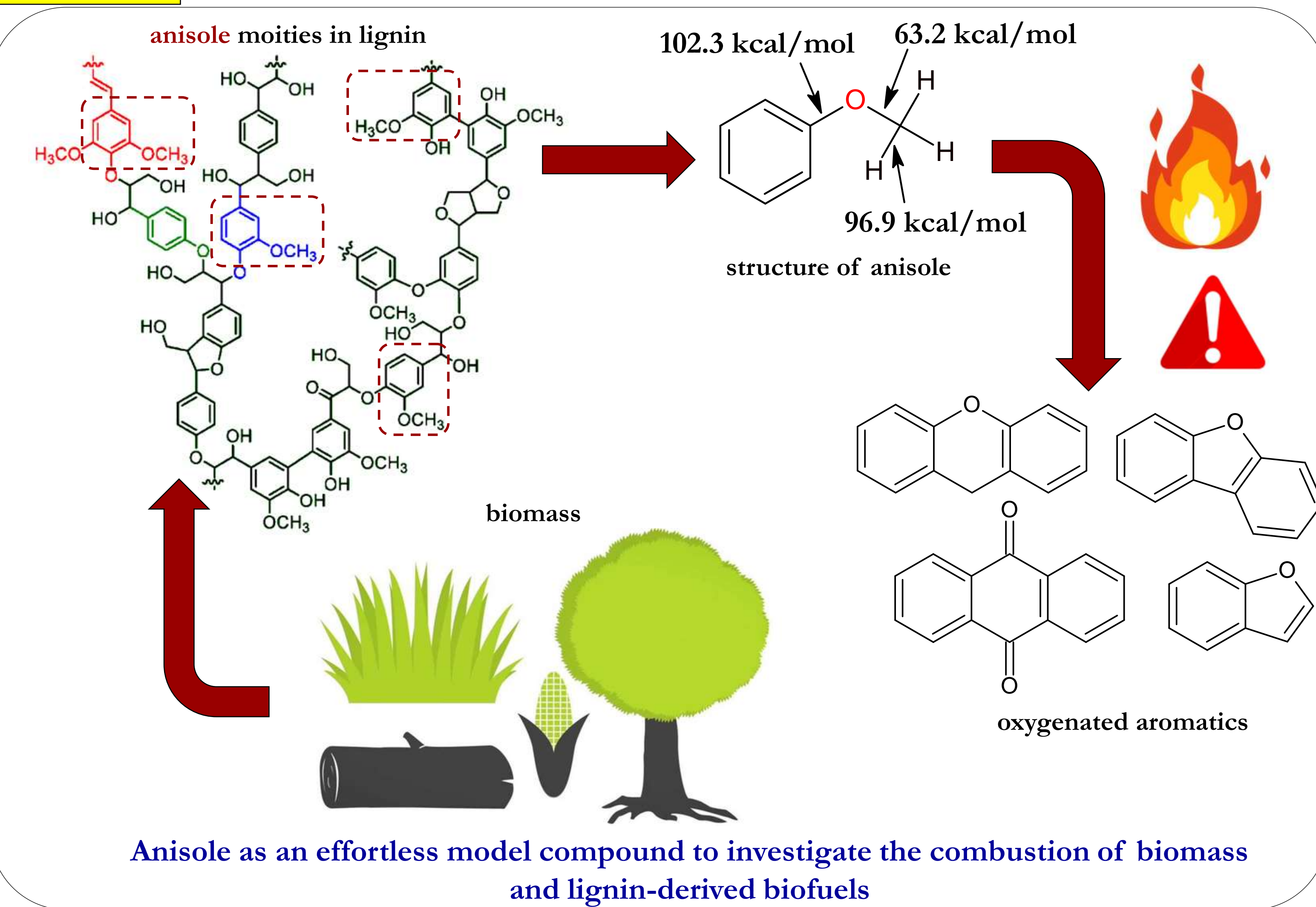
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## Context

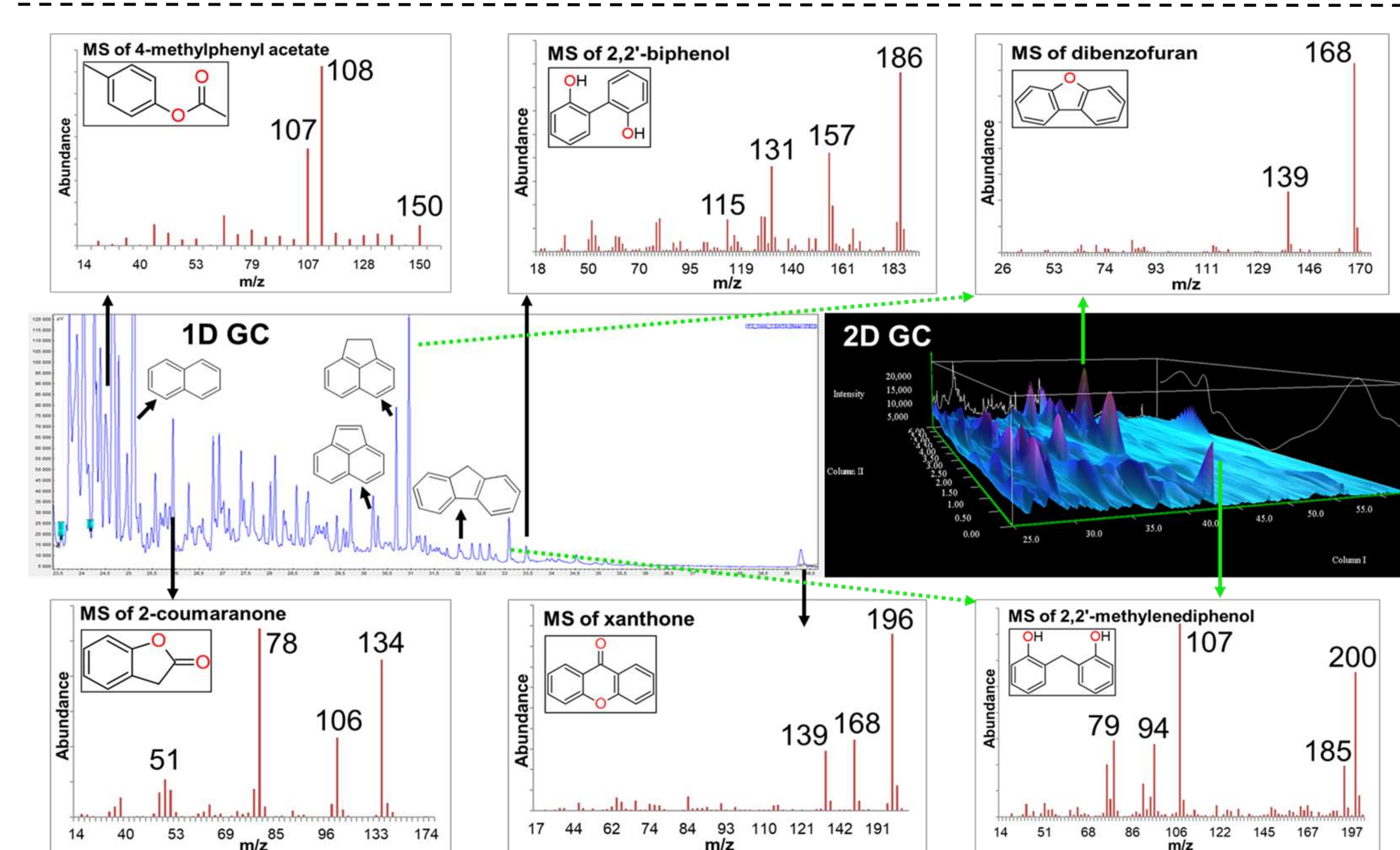
## Experimental method



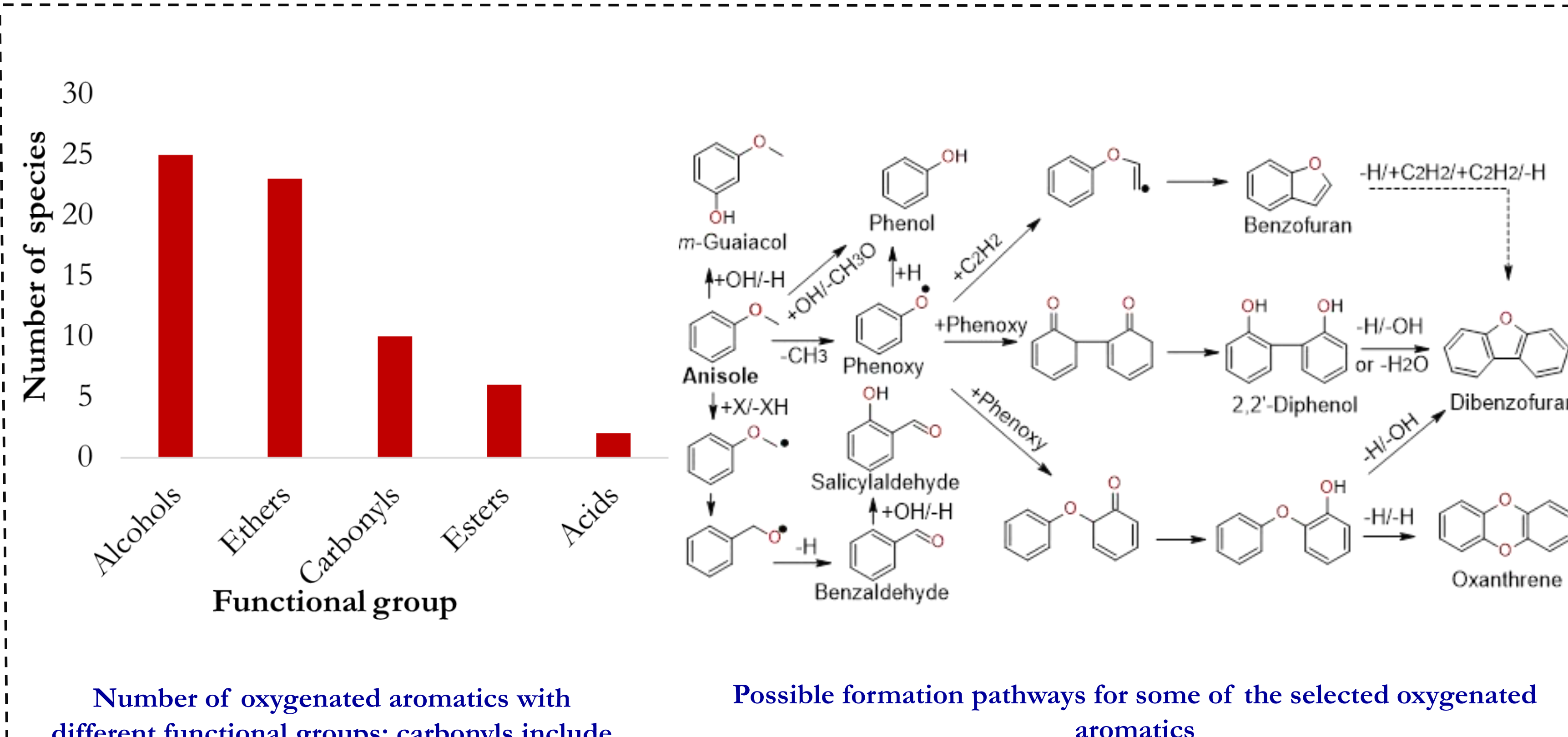
## Results

| M   | Formula  | Name  | Structure |
|-----|--|---|-----------|
| 94  | C <sub>6</sub> H <sub>6</sub> O                | Phenol  |           |
| 106 | C <sub>7</sub> H <sub>6</sub> O                | Benzaldehyde  |           |
| 108 | C <sub>7</sub> H <sub>8</sub> O                | Anisole   |           |
|     | C <sub>7</sub> H <sub>8</sub> O                | <i>o</i> -Cresol;<br>2-Methylphenol   |           |
|     | C <sub>7</sub> H <sub>8</sub> O                | <i>m</i> -Cresol;<br>3-Methylphenol   |           |
|     | C <sub>7</sub> H <sub>8</sub> O                | <i>p</i> -Cresol;<br>4-Methylphenol   |           |
| 110 | C <sub>6</sub> H <sub>6</sub> O <sub>2</sub>   | Hydroquinone;<br>Benzene-1,4-diol   |           |
| 118 | C <sub>8</sub> H <sub>6</sub> O                | Benzofuran;<br>1-Benzofuran   |           |
| 120 | C <sub>8</sub> H <sub>8</sub> O                | Dihydrobenzofuran;<br>2,3-Dihydro-1-benzofuran                              |           |
| 122 | C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>   | Salicylaldehyde;<br>2-Hydroxybenzaldehyde                                   |           |
|     | C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>   | <i>m</i> -Formylphenol;<br>3-Hydroxybenzaldehyde                            |           |
|     | C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>   | 1,3-Benzodioxole;<br>2H-1,3-benzodioxole                                    |           |
|     | C <sub>8</sub> H <sub>10</sub> O               | Ethyl phenyl ether;<br>Ethoxybenzene  |           |
|     | C <sub>8</sub> H <sub>10</sub> O               | 2,6-Xylenol;<br>2,6-Dimethylphenol  |           |
|     | C <sub>8</sub> H <sub>10</sub> O               | 2-Ethyl phenol  |           |
| 124 | C <sub>7</sub> H <sub>8</sub> O <sub>2</sub>   | <i>m</i> -Guaiaicol;<br>3-Methoxyphenol                                     |           |
| 132 | C <sub>9</sub> H <sub>8</sub> O                | 1-Indanone;<br>2,3-Dihydro-1H-inden-1-one                                   |           |
|     | C <sub>9</sub> H <sub>8</sub> O                | Cinnamaldehyde;<br>(2E)-3-Phenylprop-2-enal                                 |           |
|     | C <sub>9</sub> H <sub>8</sub> O                | 2-Methyl benzofuran;<br>2-Methyl-1-benzofuran                               |           |
| 134 | C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>   | 2-Coumaranone;<br>1-Benzofuran-2(3H)-one                                    |           |
| 136 | C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>   | <i>p</i> -Toluic acid;<br>4-Methylbenzoic acid                              |           |
|     | C <sub>9</sub> H <sub>12</sub> O               | 5-Ethyl <i>m</i> -cresol;<br>3-Ethyl-5-methylphenol                         |           |
| 144 | C <sub>10</sub> H <sub>8</sub> O               | 2-Vinyl benzofuran;<br>2-Ethynyl-1-benzofuran                               |           |
|     | C <sub>10</sub> H <sub>8</sub> O               | 1-Naphthol;<br>Naphthalen-1-ol  |           |
| 146 | C <sub>10</sub> H <sub>10</sub> O              | 1-Methylindan-2-one;<br>1-Methyl-1,3-dihydro-2H-inden-2-one                 |           |
|     | C <sub>10</sub> H <sub>10</sub> O              | 2-Ethyl benzofuran;<br>2-Ethyl-1-benzofuran                                 |           |
| 150 | C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>  | <i>o</i> -Acetoxy toluene;<br>2-Methylphenyl acetate                        |           |
|     | C <sub>9</sub> H <sub>10</sub> O <sub>2</sub>  | <i>p</i> -Acetoxy toluene;<br>4-Methylphenyl acetate                        |           |
| 156 | C <sub>11</sub> H <sub>8</sub> O               | 2-Naphthaldehyde;<br>Naphthalen-2-carbaldehyde                              |           |
| 162 | C <sub>11</sub> H <sub>14</sub> O              | 2,2-dimethyl-3,4-dihydro-2H-1-Benzopyran                                    |           |
| 168 | C <sub>12</sub> H <sub>8</sub> O               | Dibenzofuran;<br>Dibenzo[ <i>b,d</i> ]furan                                 |           |
| 170 | C <sub>12</sub> H <sub>10</sub> O              | Diphenyl ether;<br>1,1'-Oxydibenzene  |           |
|     | C <sub>12</sub> H <sub>10</sub> O              | Hydroxybiphenyl;<br>[1,1'-Biphenyl]-2-ol                                    |           |
|     | C <sub>12</sub> H <sub>10</sub> O              | 1-Naphthyl vinyl ether;<br>1-(Ethenyloxy)naphthalene                        |           |
| 180 | C <sub>13</sub> H <sub>8</sub> O               | 9-Fluorenone;<br>9H-Fluoren-9-one   |           |
| 182 | C <sub>13</sub> H <sub>10</sub> O              | Xanthene;<br>9H-Xanthene  |           |
|     | C <sub>13</sub> H <sub>10</sub> O              | 9-Fluorenyl;<br>9H-Fluoren-9-yl   |           |
|     | C <sub>13</sub> H <sub>10</sub> O              | 4-Methylidibenzo[ <i>b,d</i> ]furan   |           |
|     | C <sub>13</sub> H <sub>10</sub> O              | 6H-Dibenzo[ <i>b,d</i> ]pyran   |           |
| 184 | C <sub>12</sub> H <sub>8</sub> O <sub>2</sub>  | Dibenzo- <i>p</i> -dioxin;<br>Oxanthrene                                    |           |
|     | C <sub>12</sub> H <sub>8</sub> O <sub>2</sub>  | 2-Dibenzofuranol;<br>Dibenzo[ <i>b,d</i> ]furan-2-ol                        |           |
|     | C <sub>13</sub> H <sub>12</sub> O              | Benzyl phenyl ether;<br>(Benzoyloxy)benzene                                 |           |
|     | C <sub>13</sub> H <sub>12</sub> O              | <i>o</i> -Benzylphenol;<br>2-Benzylphenol                                   |           |
|     | C <sub>13</sub> H <sub>12</sub> O              | <i>p</i> -Benzylphenol;<br>4-Benzylphenol                                   |           |
| 186 | C <sub>12</sub> H <sub>10</sub> O <sub>2</sub> | Diphenyl ether;<br>[1,1'-Biphenyl]-2,2'-diol                                |           |
|     | C <sub>12</sub> H <sub>10</sub> O <sub>2</sub> | <i>m</i> -Phenoxy phenol;<br>3-Phenoxyphenol                                |           |
|     | C <sub>12</sub> H <sub>10</sub> O <sub>2</sub> | 1-Naphthyl acetate;<br>Naphthalen-1-yl acetate                              |           |
|     | C <sub>13</sub> H <sub>14</sub> O              | 2-((2-Naphthyl)-2-propanol);<br>2-(Naphthalen-2-yl)propan-2-ol              |           |
|     | C <sub>13</sub> H <sub>14</sub> O              | 2,5,8-Trimethylnaphthalen-1-ol  |           |
| 196 | C <sub>13</sub> H <sub>8</sub> O <sub>2</sub>  | Xanthone;<br>9H-Xanthen-9-one   |           |
| 198 | C <sub>14</sub> H <sub>14</sub> O              | 1,2,3,4-tetrahydrophenanthren-4-ol  |           |
|     | C <sub>13</sub> H <sub>12</sub> O <sub>2</sub> | Bis(2-hydroxyphenyl) methane;<br>2,2'-Methylenediphenol                     |           |
|     | C <sub>13</sub> H <sub>12</sub> O <sub>2</sub> | 2-((4-Hydroxyphenyl)methyl)phenol   |           |
| 208 | C <sub>14</sub> H <sub>8</sub> O <sub>2</sub>  | Anthraquinone;<br>Anthracen-9,10-dione                                      |           |
| 212 | C <sub>15</sub> H <sub>16</sub> O              | 1,1-Diphenyl-1-methoxyethane;<br>1,1'-(1-Methoxyethane-1,1-diylo) dibenzene |           |
| 224 | C <sub>15</sub> H <sub>12</sub> O <sub>2</sub> | 9-Fluorenyl acetate;<br>9H-Fluoren-9-yl acetate                             |           |
| 226 | C <sub>14</sub> H <sub>10</sub> O <sub>3</sub> | Xanthene-9-carboxylic acid;<br>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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