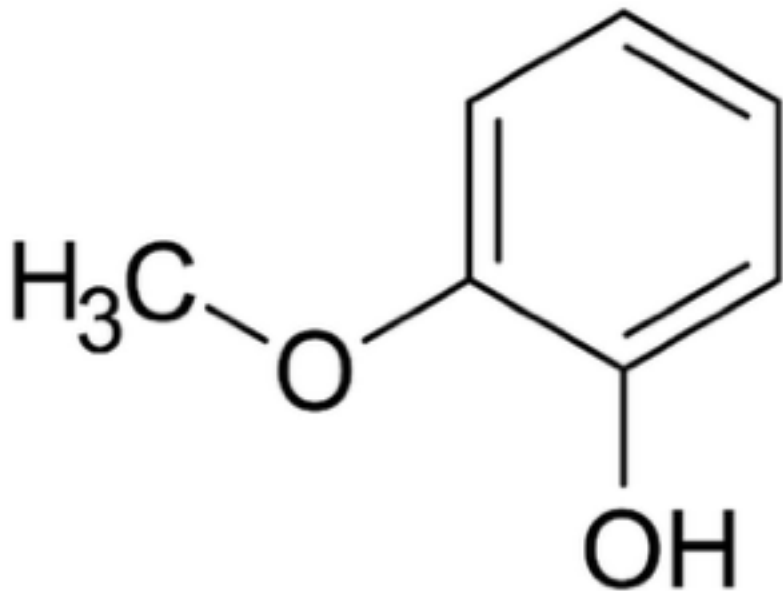


Noncurses

• Water

• Ethanol

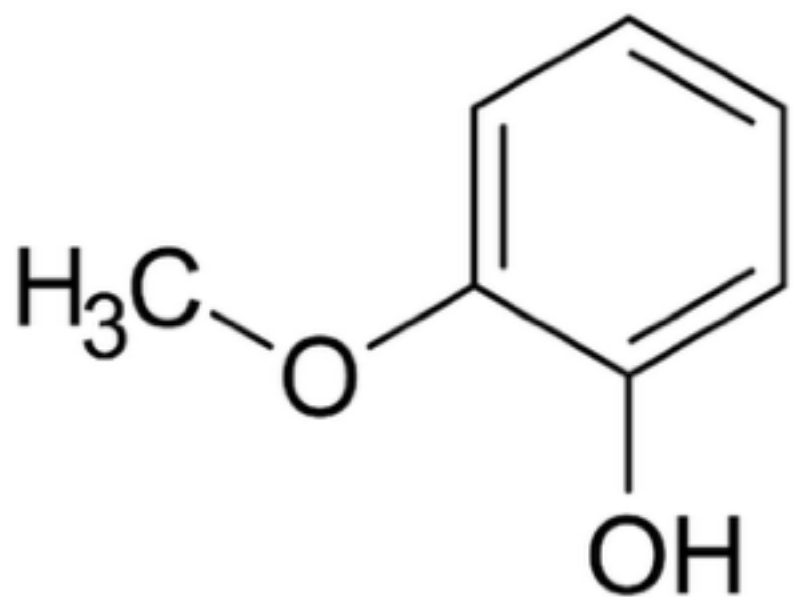
• Guaiacol (2-methoxyphenol)



- Flavor component in Scotch whisky, especially peated (high phenol) such as Islay (Ardbeg, Laphroaig, Lagavulin)
- Active ingredient in anti-cough solution Pulmo Bailey


Molecules

- Water
- Ethanol
- Guaiacol (2-methoxy phenol)



- Flavor component in Scotch whisky, especially peated (high phenol) such as Islay (Ardbeg, Laphroaig, Lagavulin)
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Methods

- Optimize model for guaiacol
 - HF/6-31G* 
- Molecular dynamics
 - GAFF, AMBER12SB, SPC/E
 - Bulk (NPT)
 - Extended box with interface (NVT)