



Computational Physics Course

Learn to use software packages

Home

More

1. Install software

There are several ways to prepare your computational environment in your laptop PC.

1. Use [Materiapps](#).
2. Use virtual machine (VMware or Virtual Box) and install LINUX (ubuntu), where packages are to be installed.
3. Use your own way.

I recommend you to follow both 1 and 2 if you are not so familiar with computers.



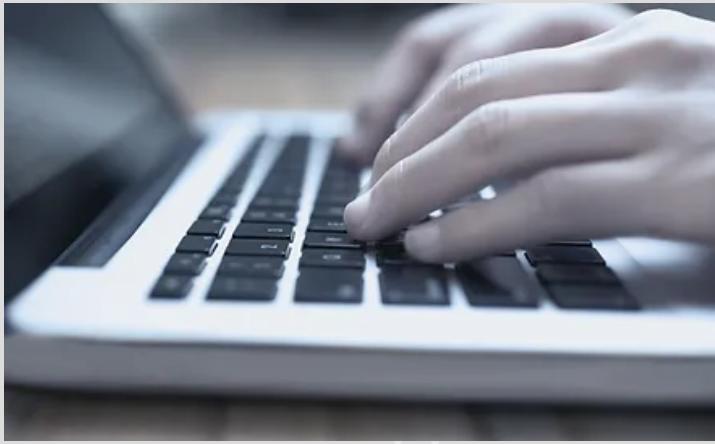
What can we do with Materiapps?

What is Materiapps?

By clicking "tryout applications" in [Materiapps](#), you are lead to the introduction page. You can see the video indicating how to start Materiapps Live and how to use a package "Tapioca", with which to analyze your input and output files. In addition, you will find many packages in the web site indicating that this is a portal site.

Using the computational environment provided by Materiapps Live, you can easily start learning. The easiest way will be to use the USB memory for Materiapps Live; you can see the video for instruction.

Some of the packages are already installed, but most of them require your effort to install. Installation is, in general, not so difficult. But there may be cases that require certain level of knowledge on LINUX, but do not worry about it: You might solve the problem by using the apt command.



In addition, let us install the followings:

- build essential, gfortran, fftw3-dev

```
sudo apt-get install essential
```

```
sudo apt-get install gfortran
```

```
sudo apt-get install fftw3-dev
```

- vmd

Visit the site

<http://www.ks.uiuc.edu/Research/vmd/>
and follow the instruction

- LAPACK

- Download package from

<http://www.netlib.org/lapack/>

- unpack the tgz file using the command "tar - xzvf". Then you will see a newly constructed directory lapack-3.6.1

- cd lapack-3.6.1

- cp make.inc.example make.inc

- make blaslib

- make lapacklib

- make tmglib

- sudo cp librefblas.a /usr/local/lib/libblas.a

- sudo cp liblapack.a /usr/local/lib/liblapack.a

- sudo cp libtmglib.a /usr/local/lib/libtmgl.a



Preparing ubuntu environment

1. Install VMware player (free) from

<http://www.vmware.com>

2. Install ubuntu into VMware.

- Download ubuntu from

<https://www.ubuntu.com/desktop>

- Use installer of VMware. Follow instruction appearing in a web site.

3. Install Quantum Espresso

- (a) From terminal of ubuntu type

```
sudo apt-get install quantum-espresso
```

Then, version 5.1 of Quantum Espresso (QE) is available.

- (b) Install also xcrysden and gnuplot by typing

```
sudo apt-get install xcrysden
```

```
sudo apt-get install gnuplot
```

For the steps 1 and 2, you can see youtube videos (shown below) for detailed instruction.

We will used this software

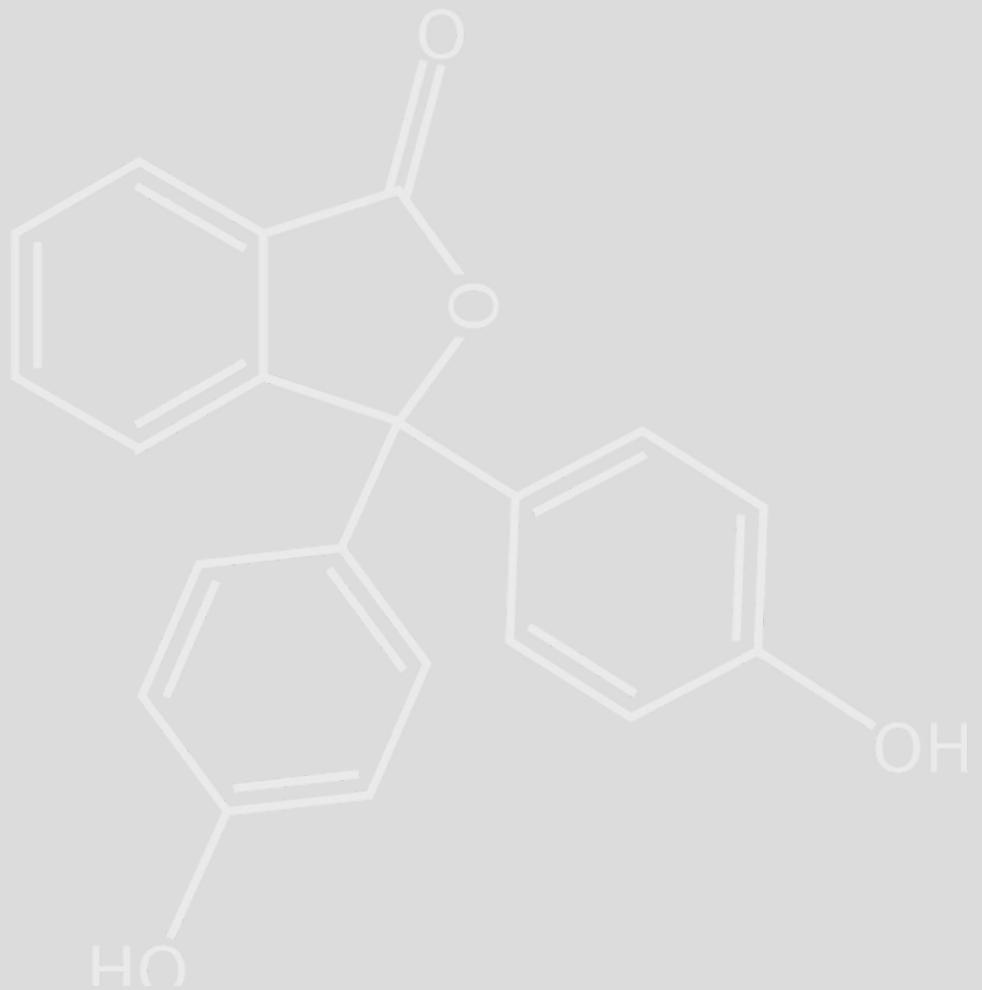
Now you have installed the minimal environment.

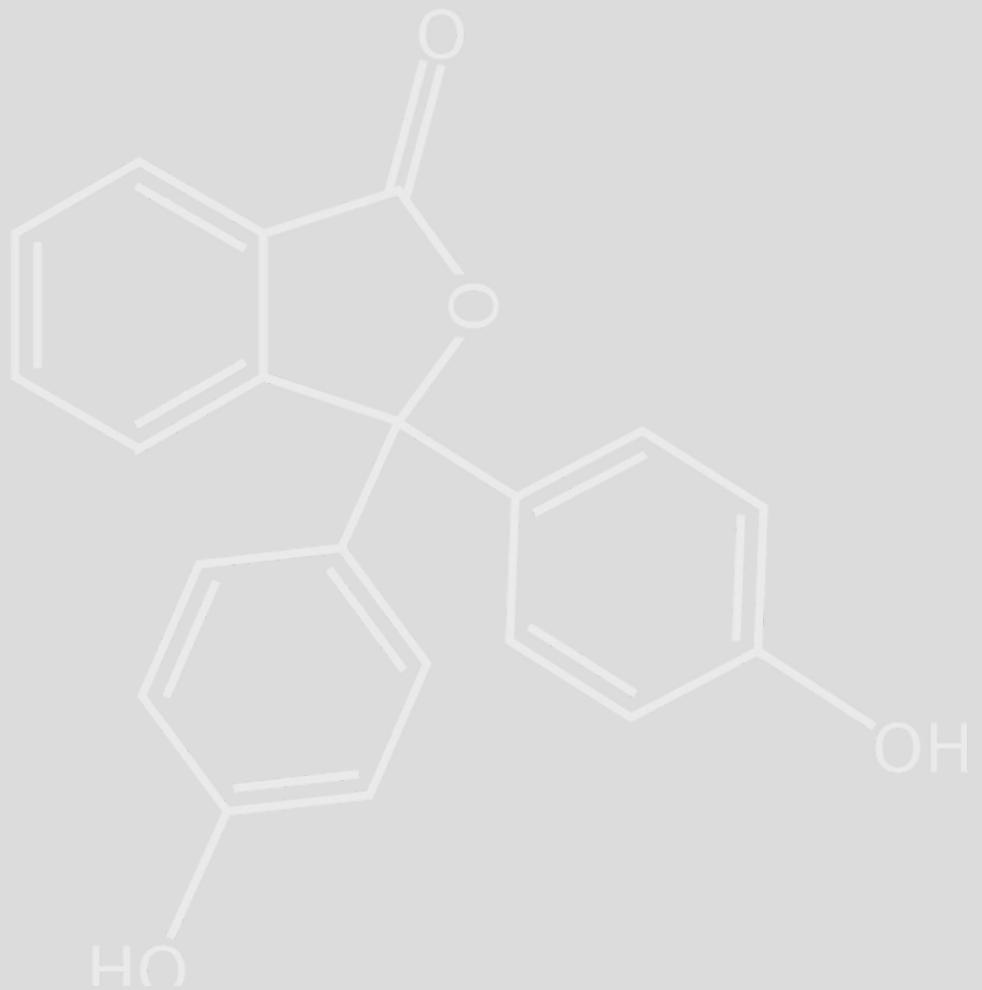
[How to install VMware Workstation...](#)

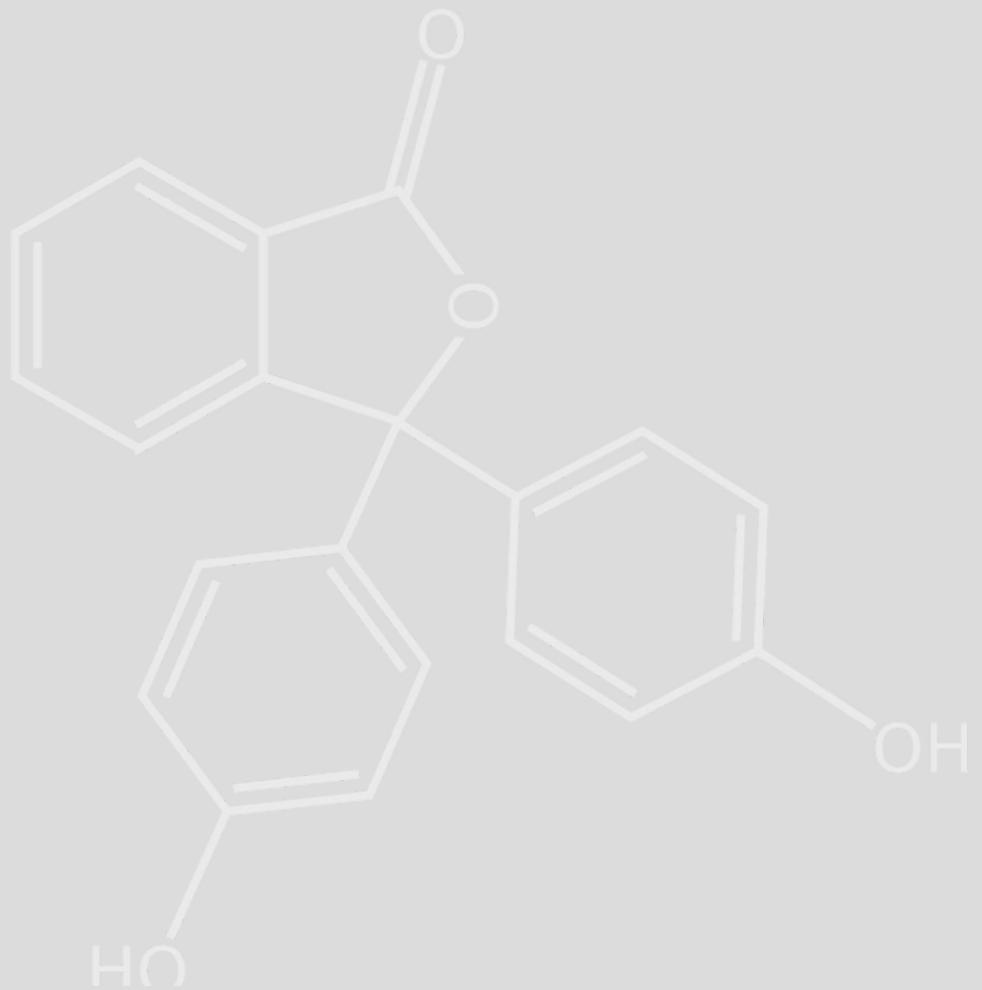


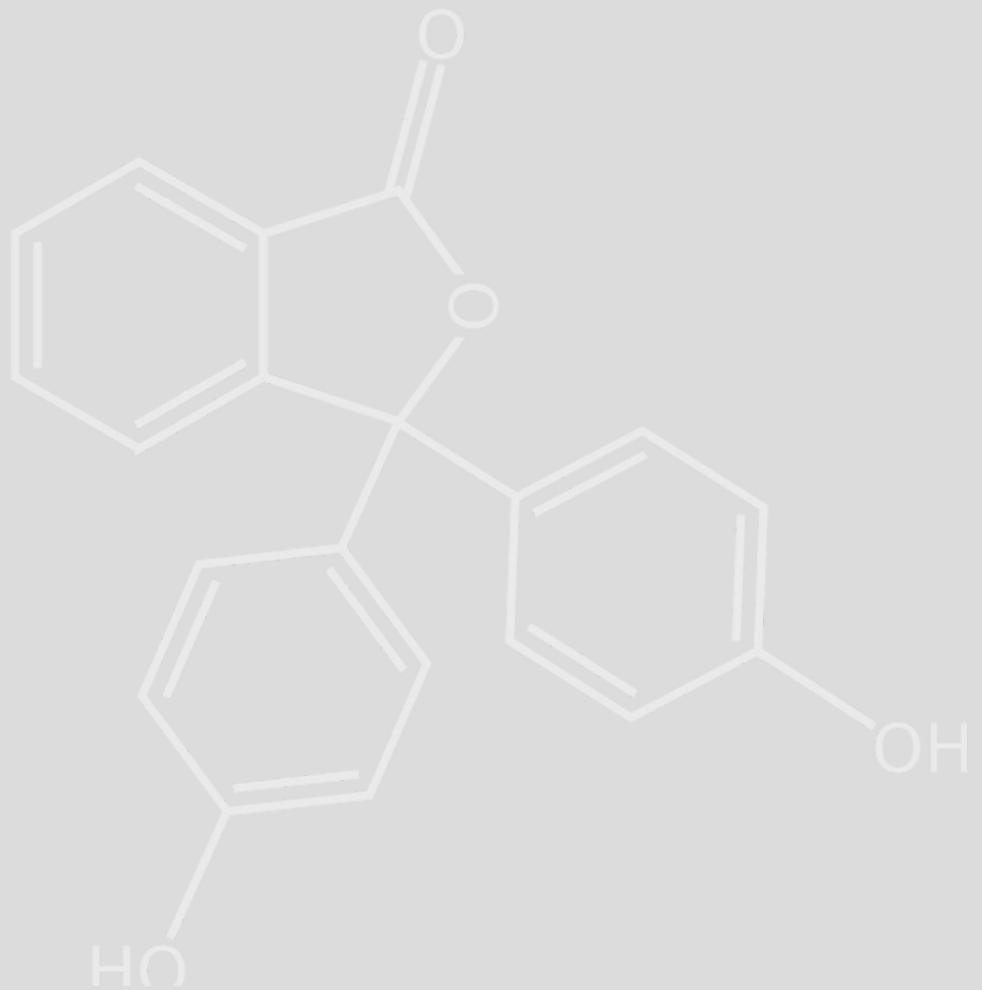
[How to install Ubuntu 15 \(using ...](#)

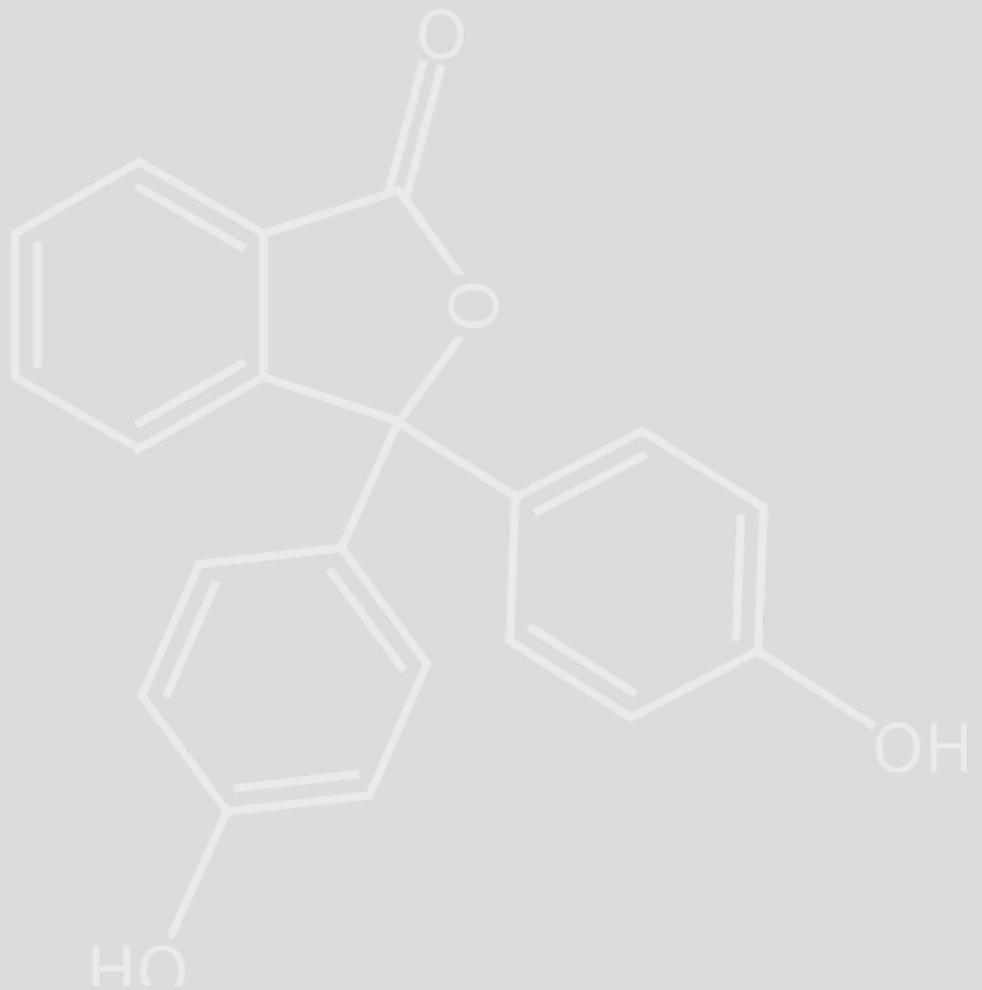


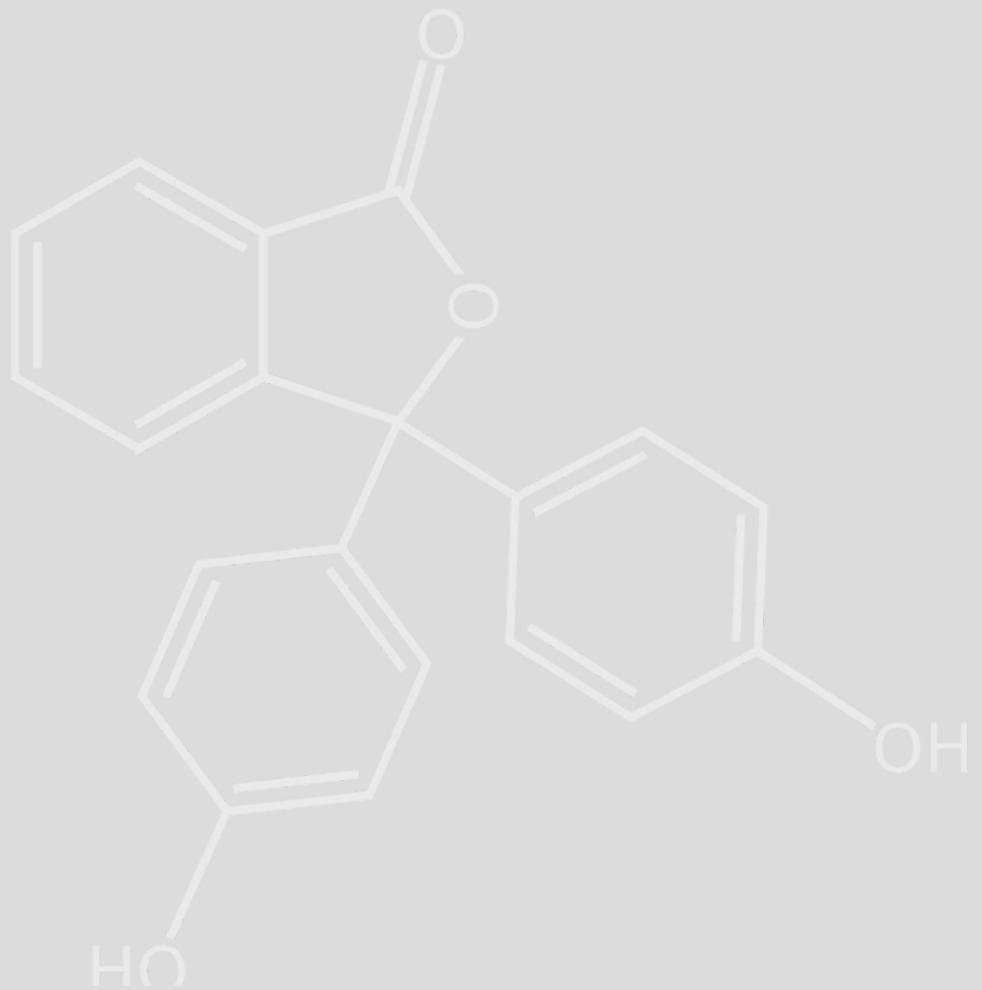


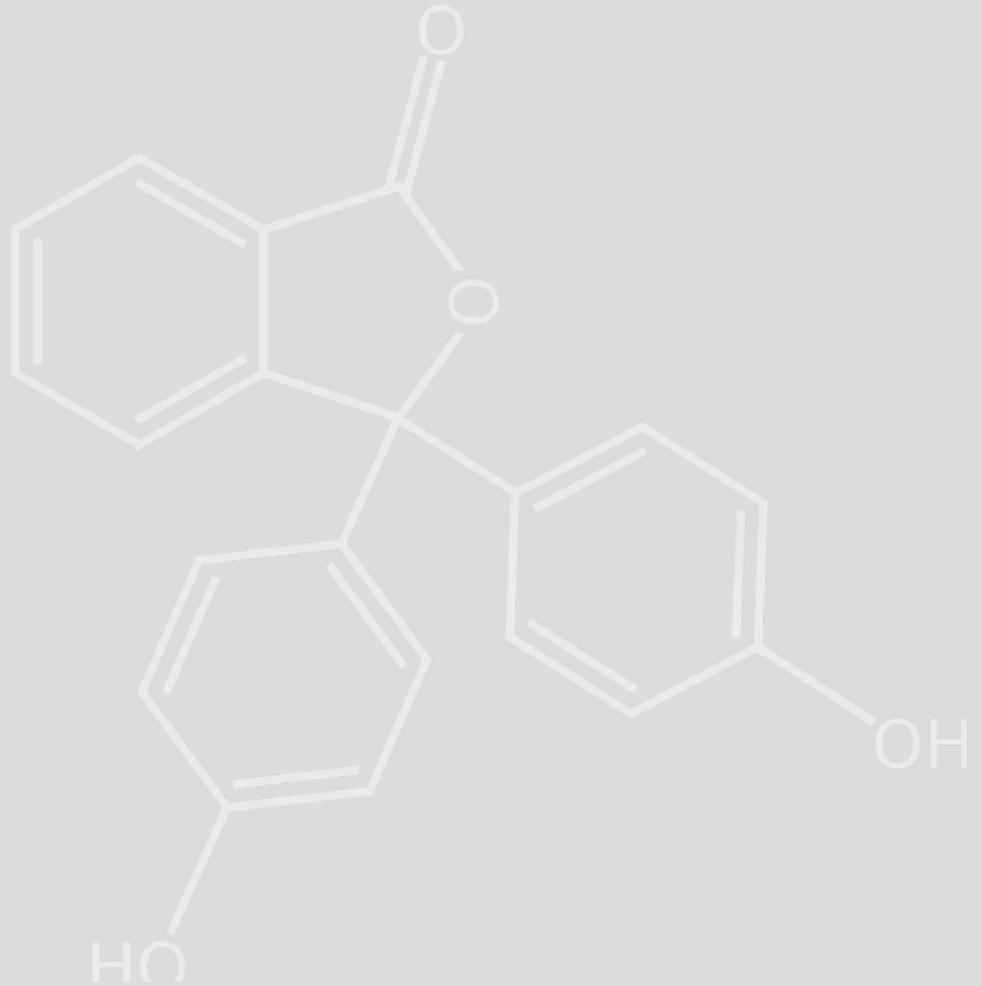


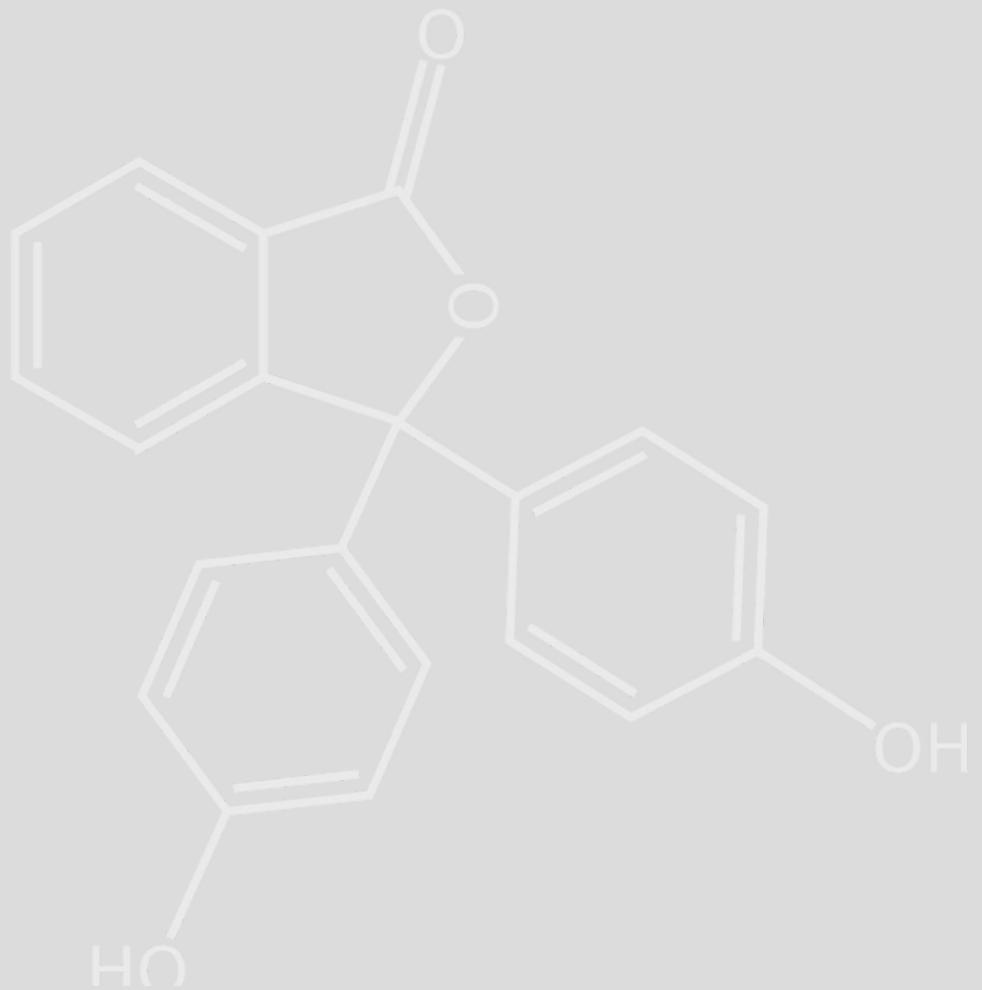


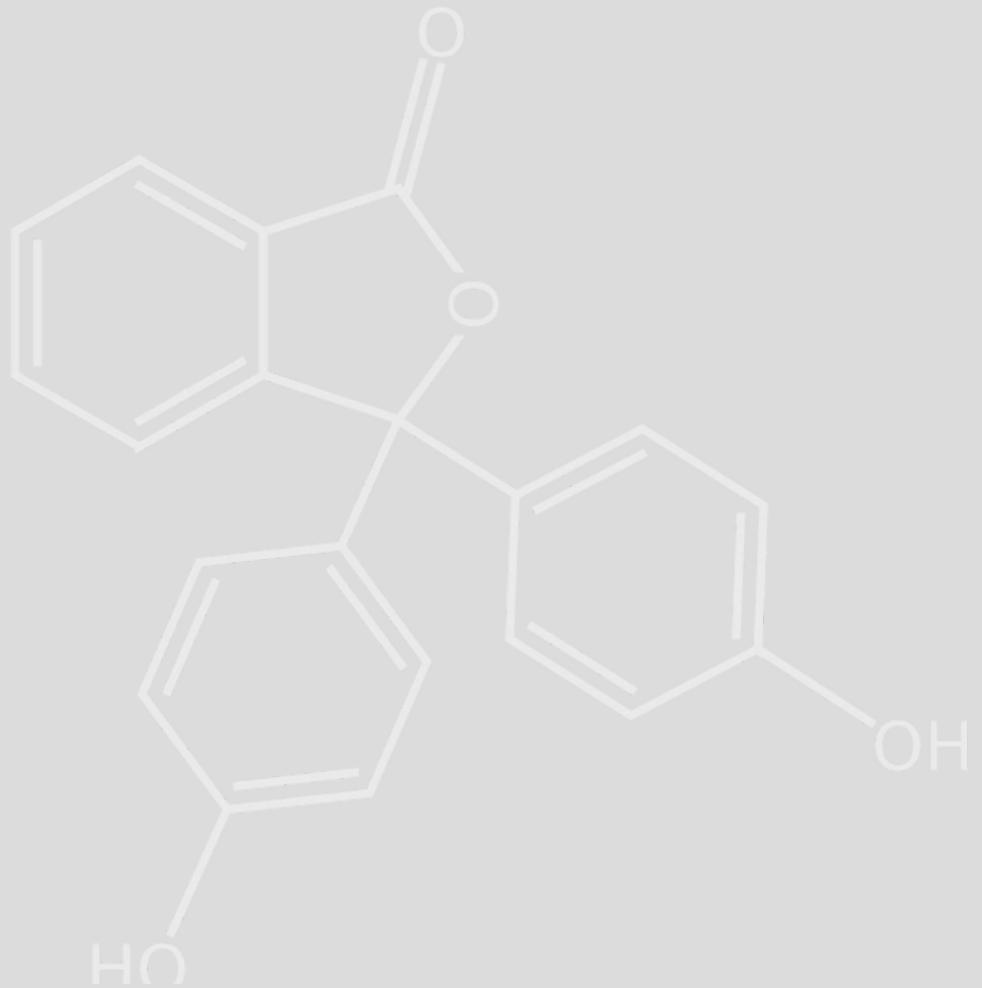


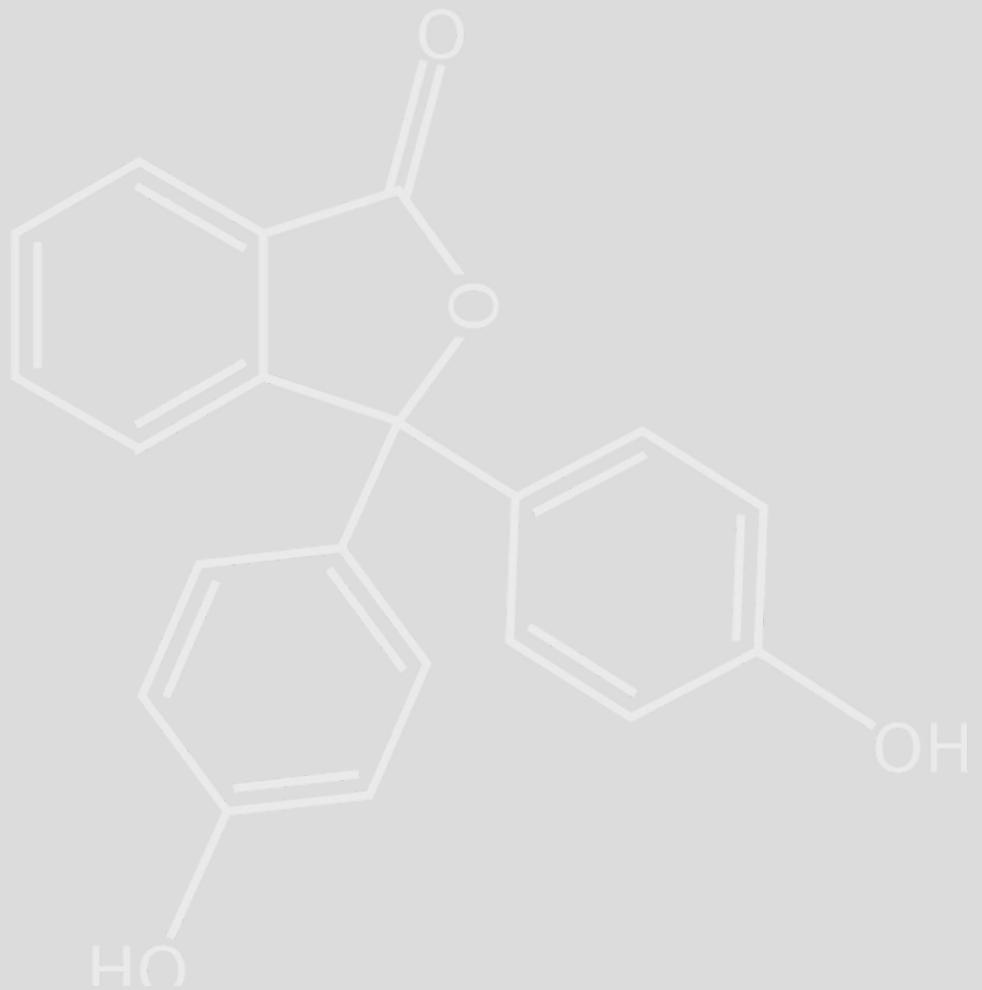


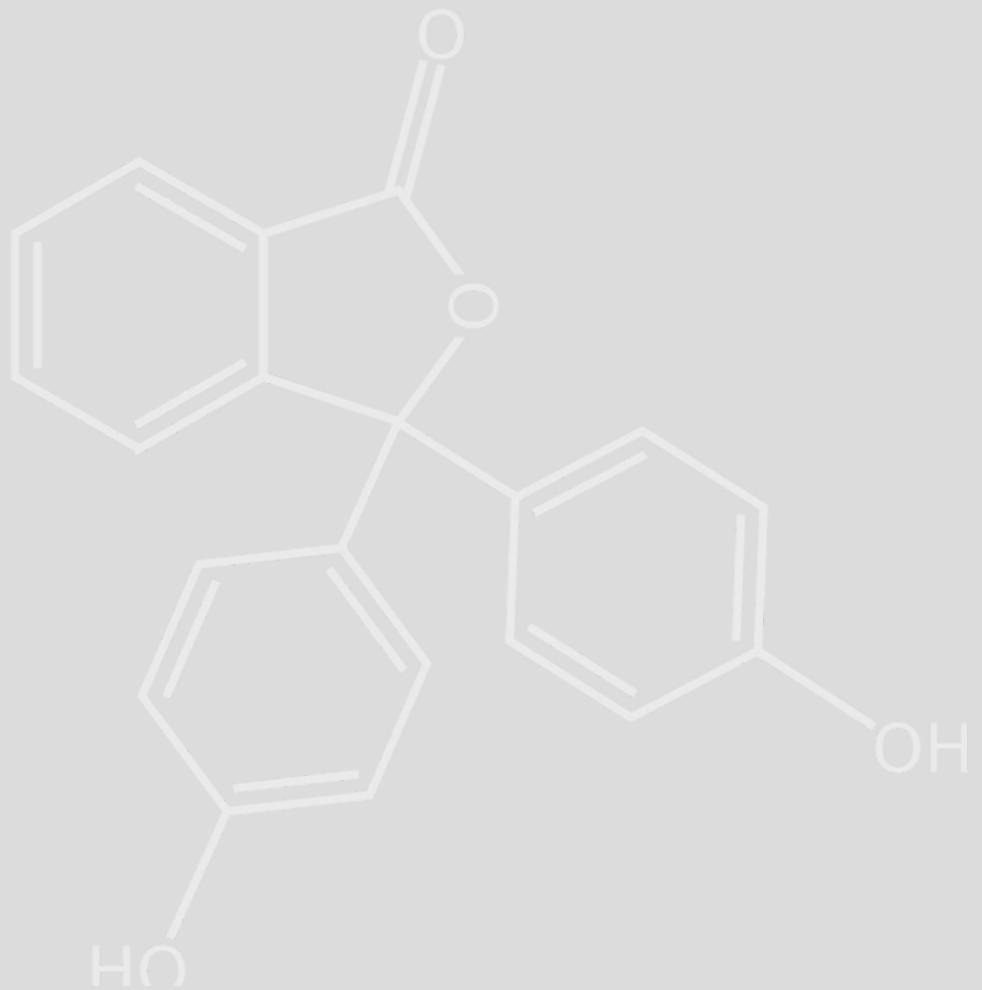


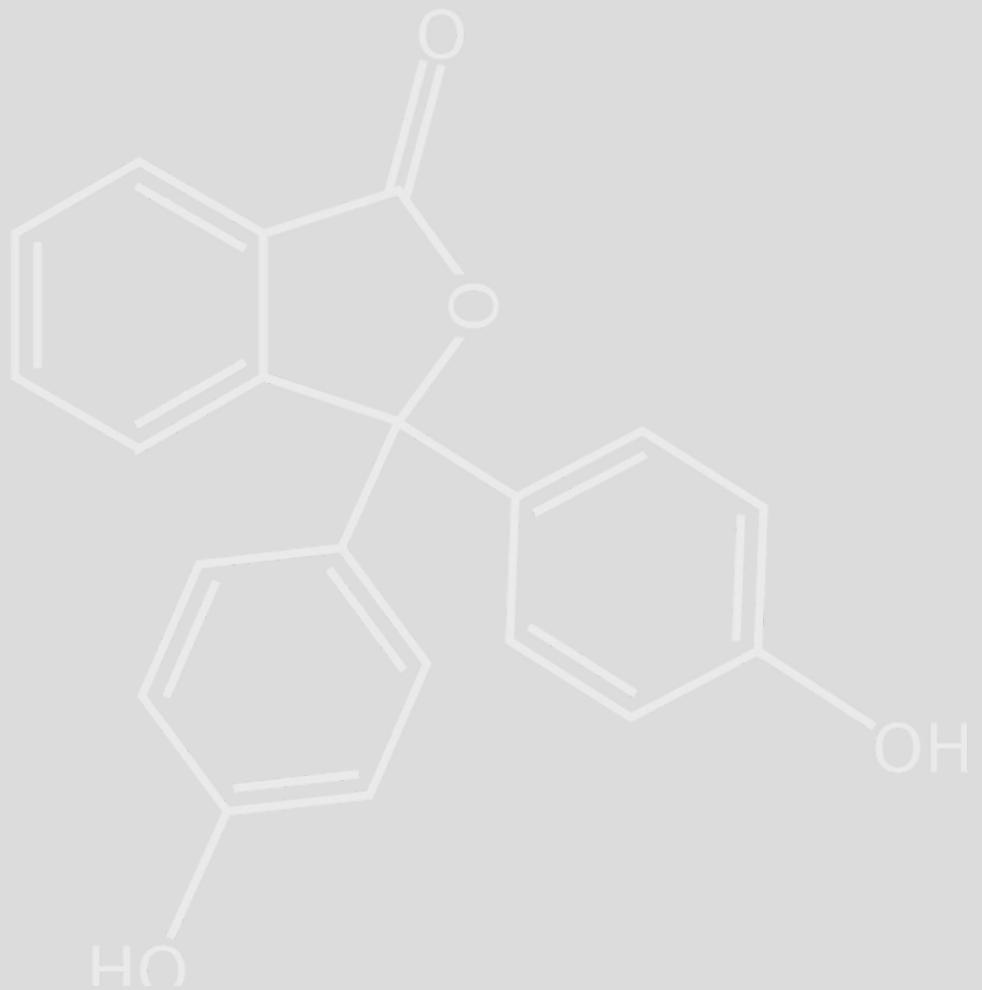


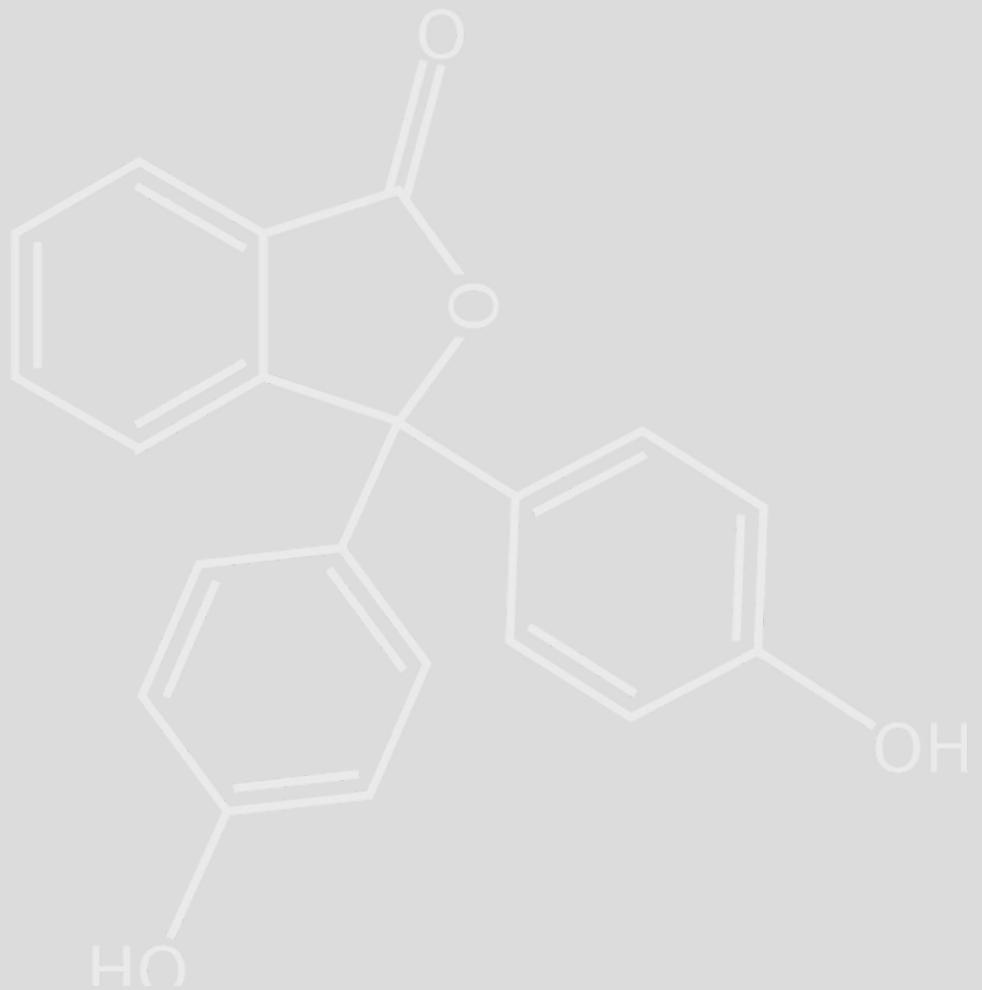


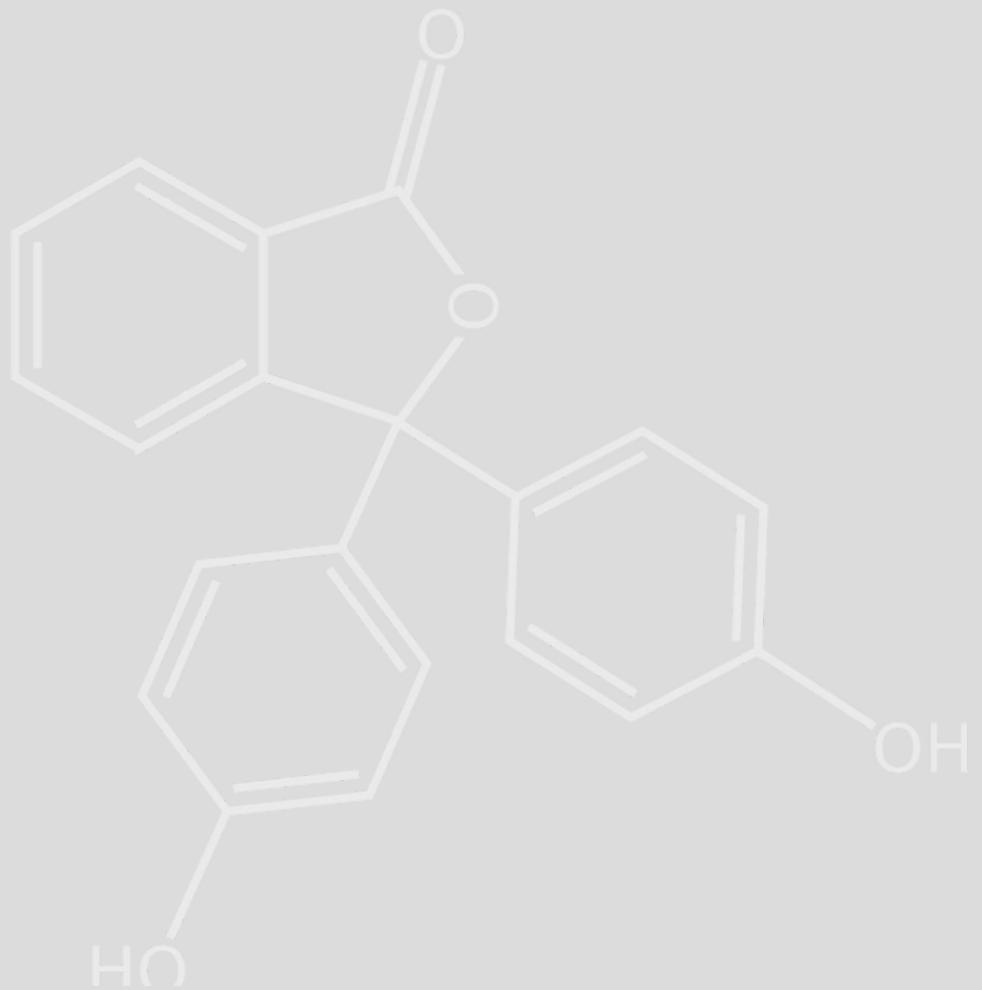


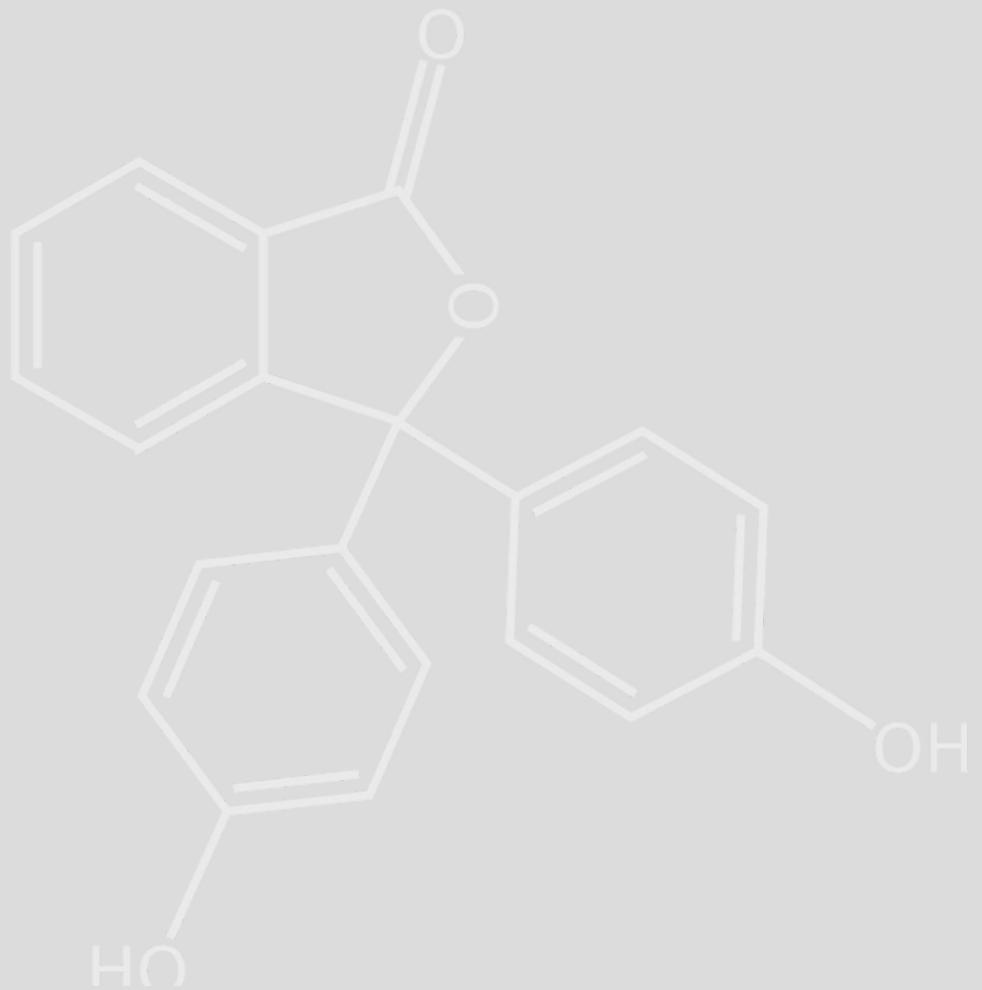


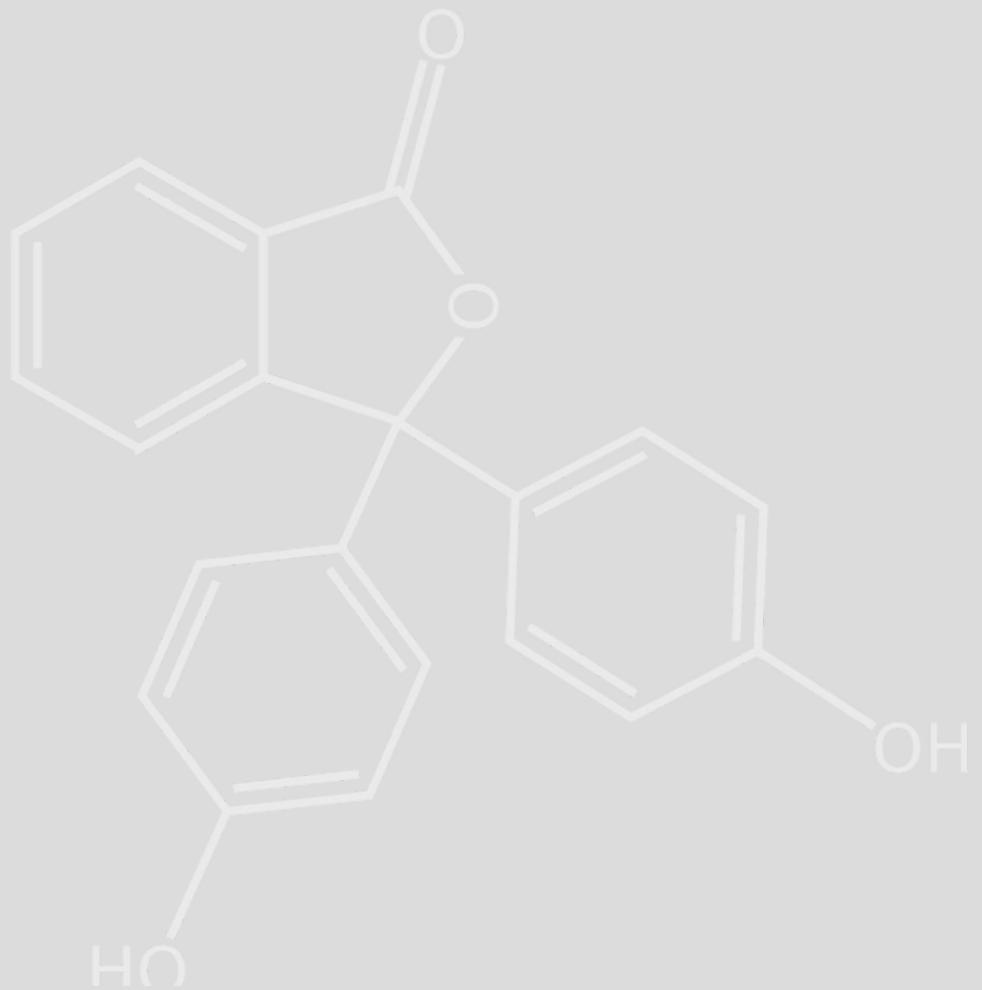


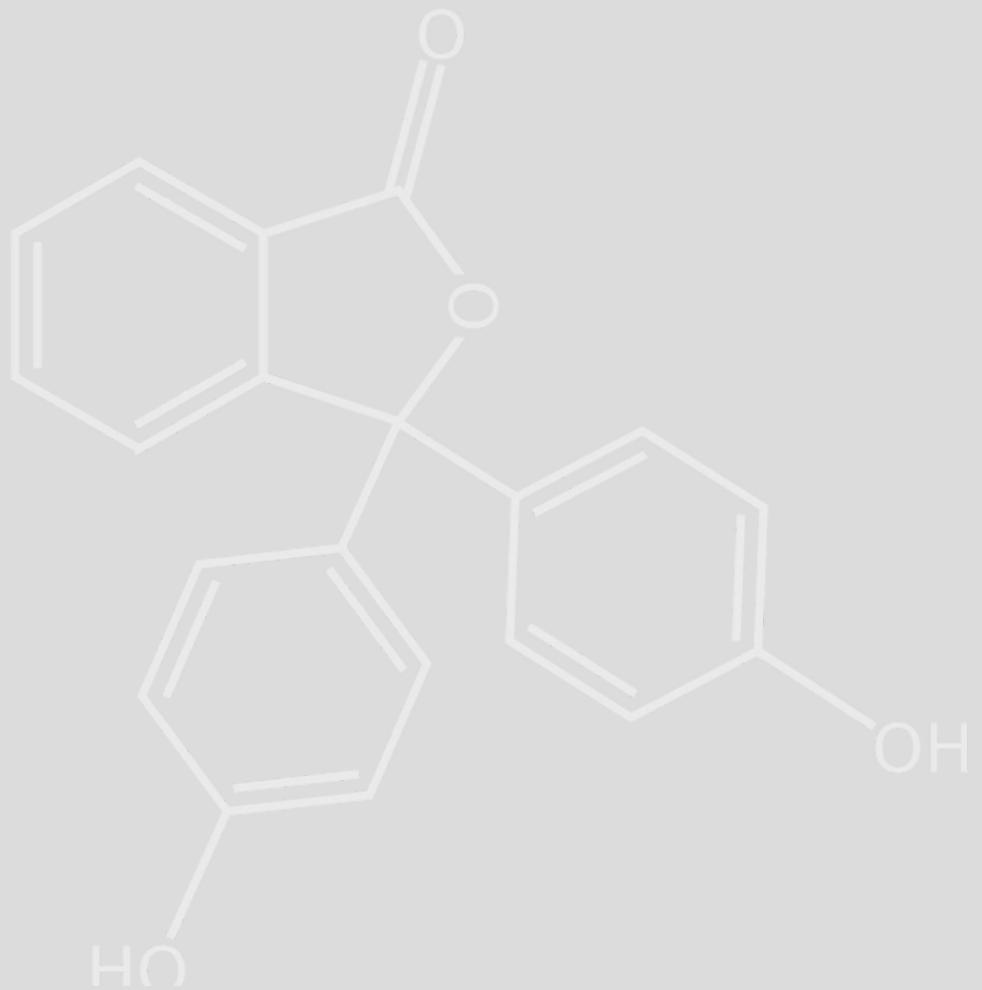


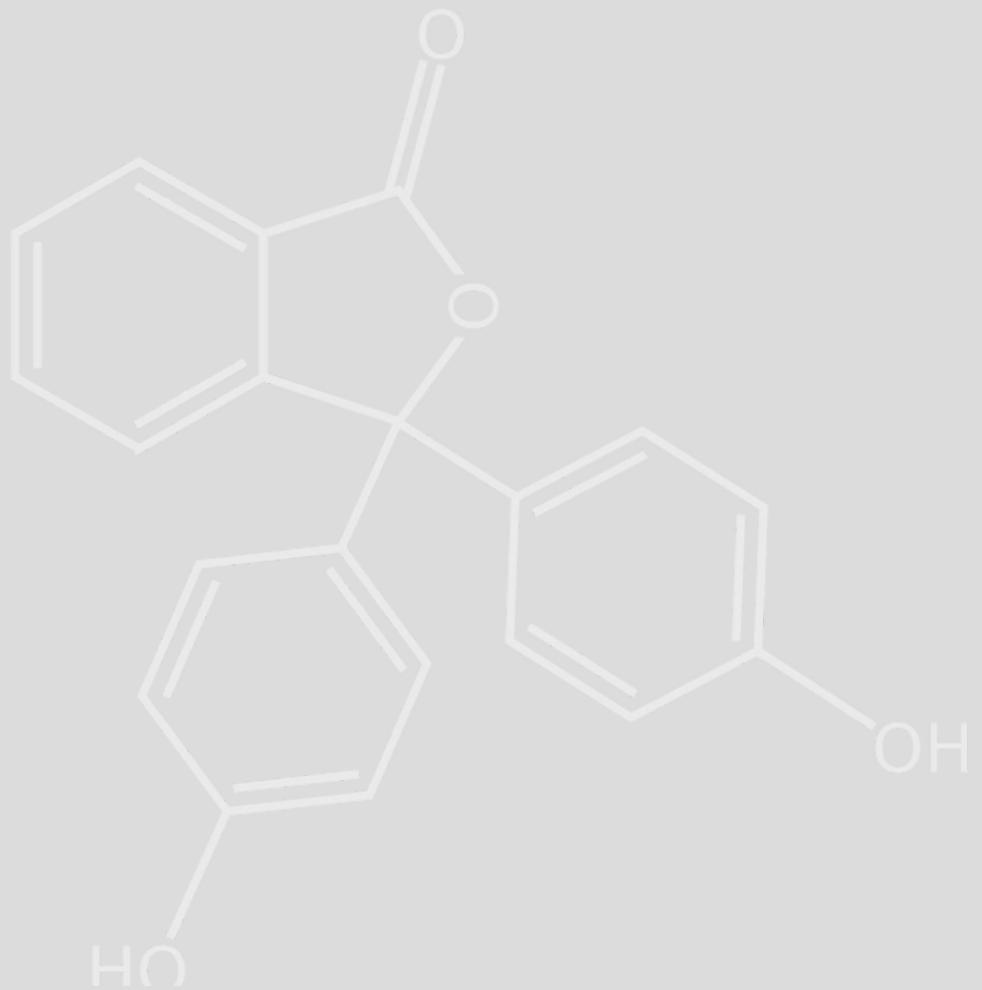


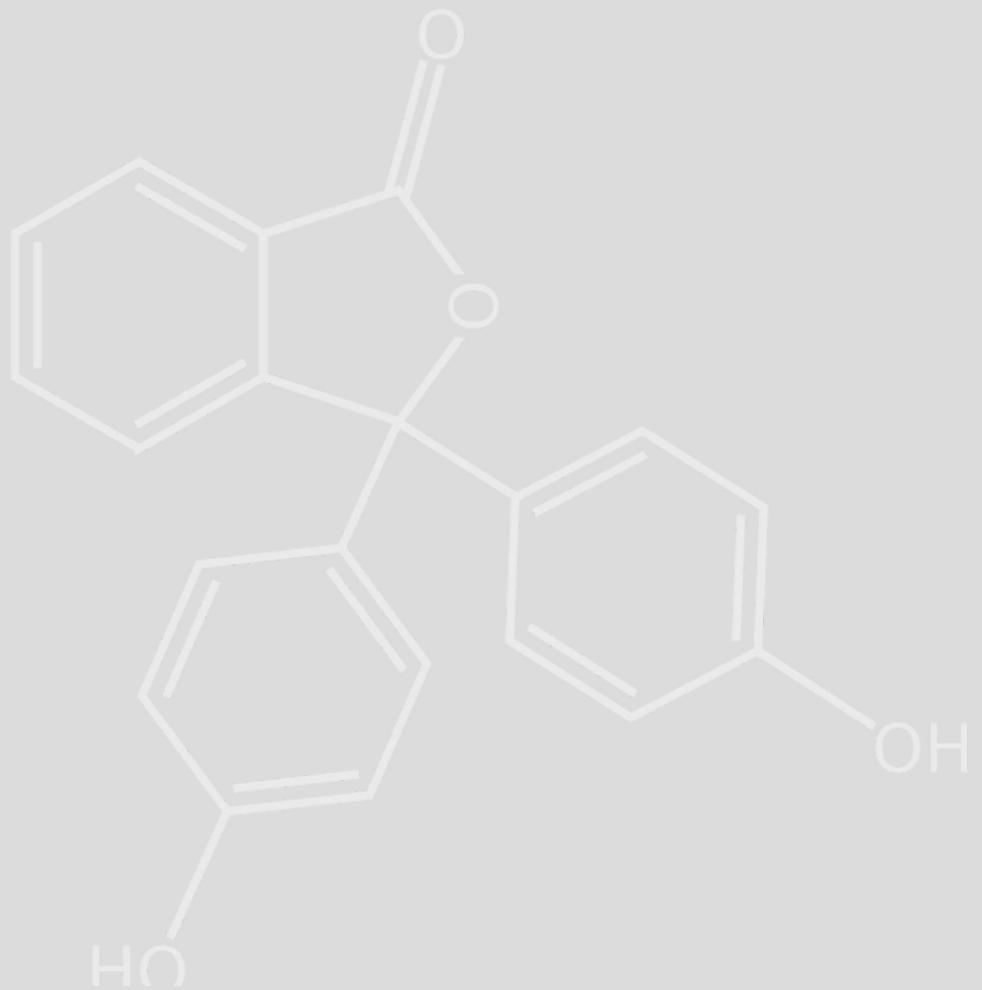


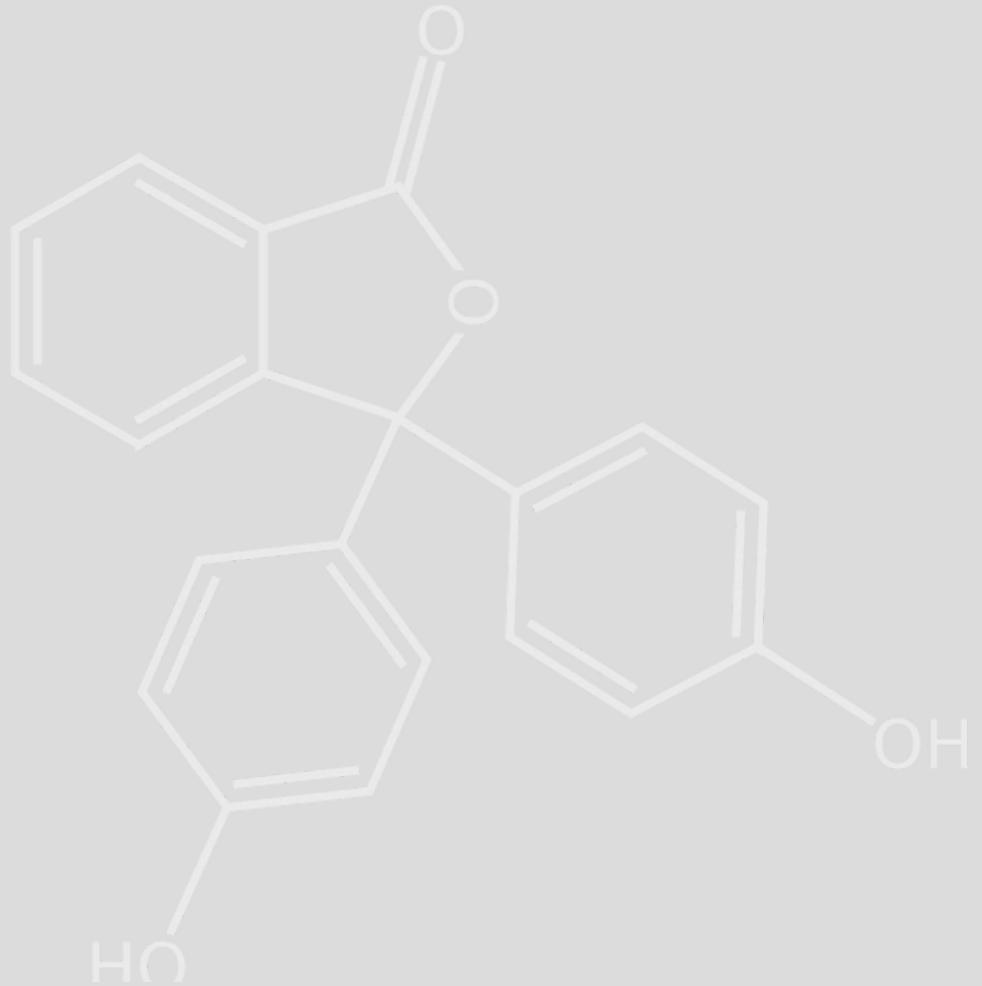


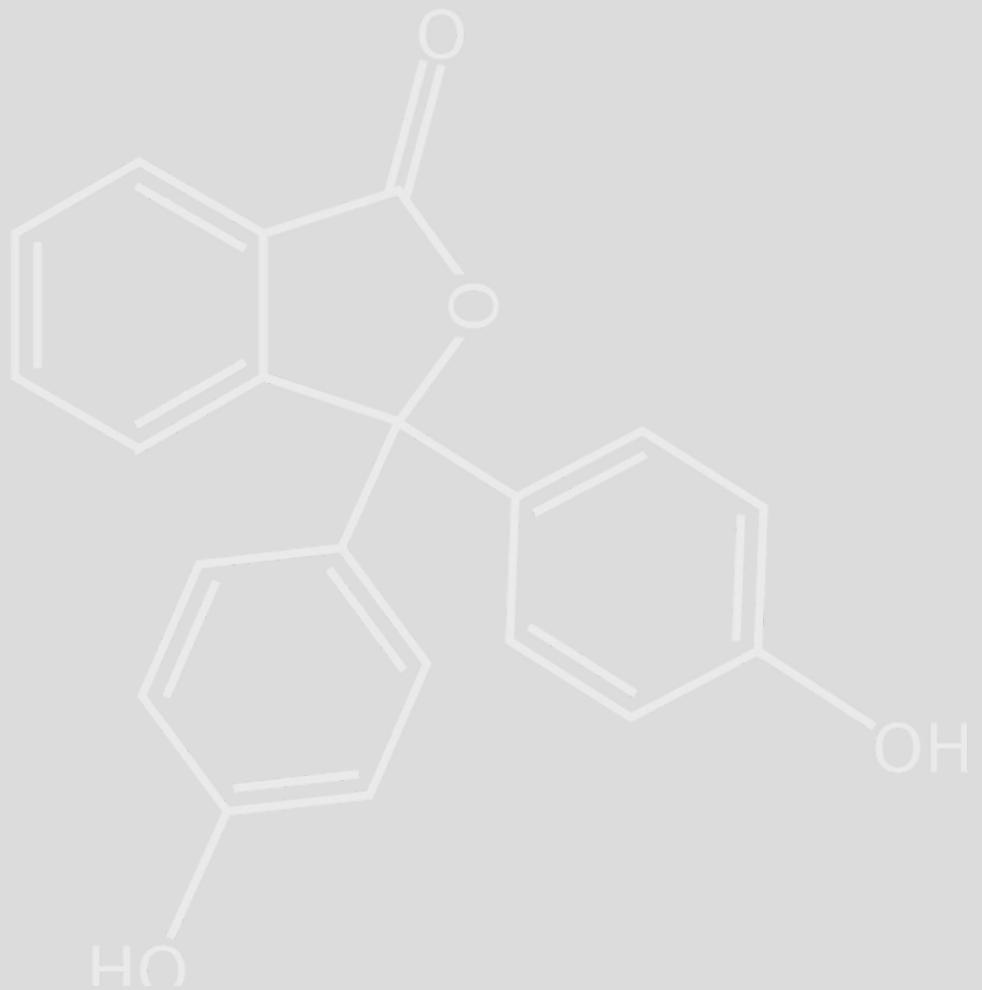


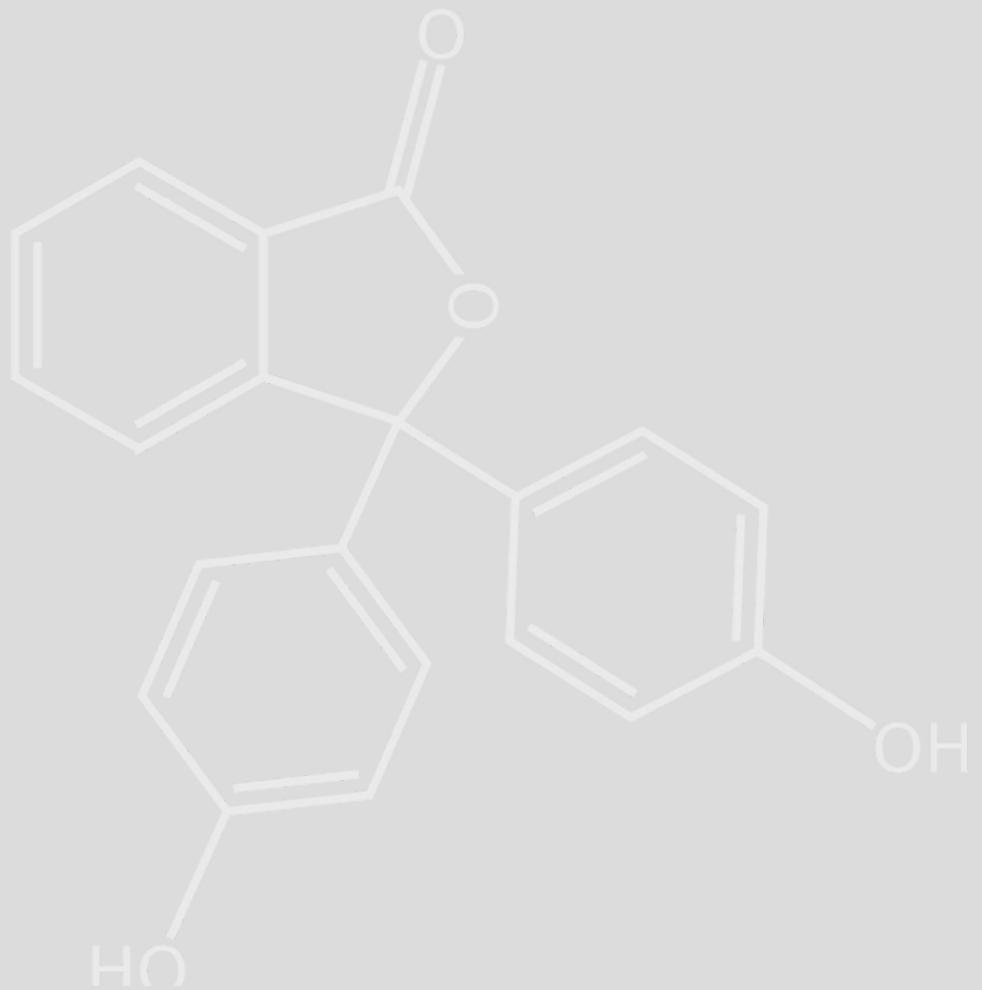


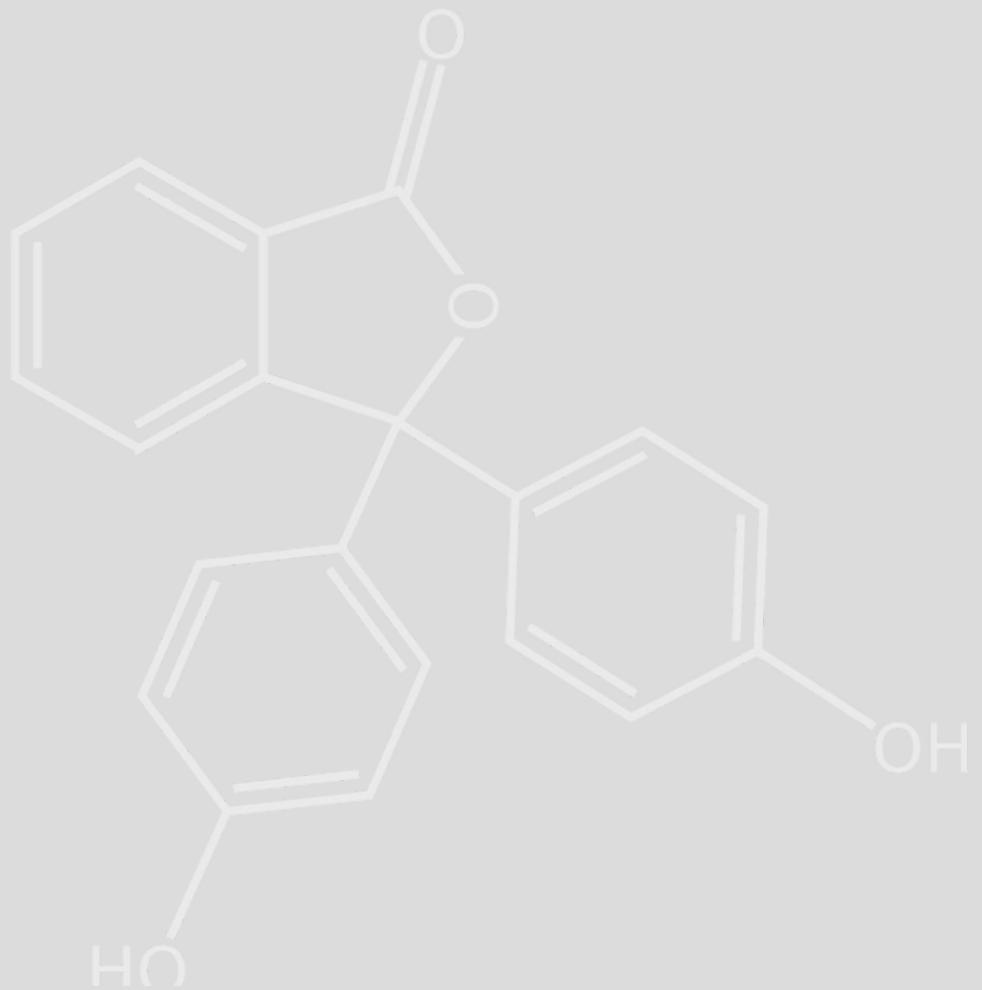


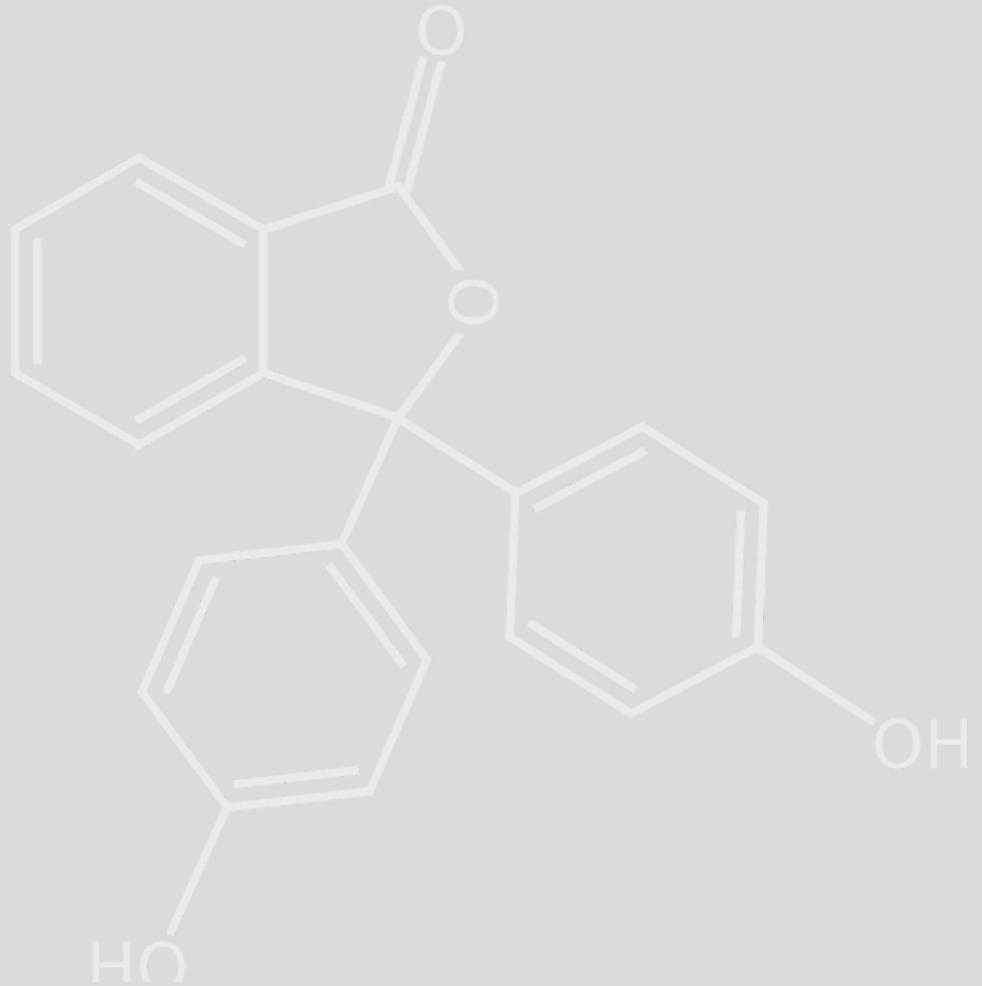


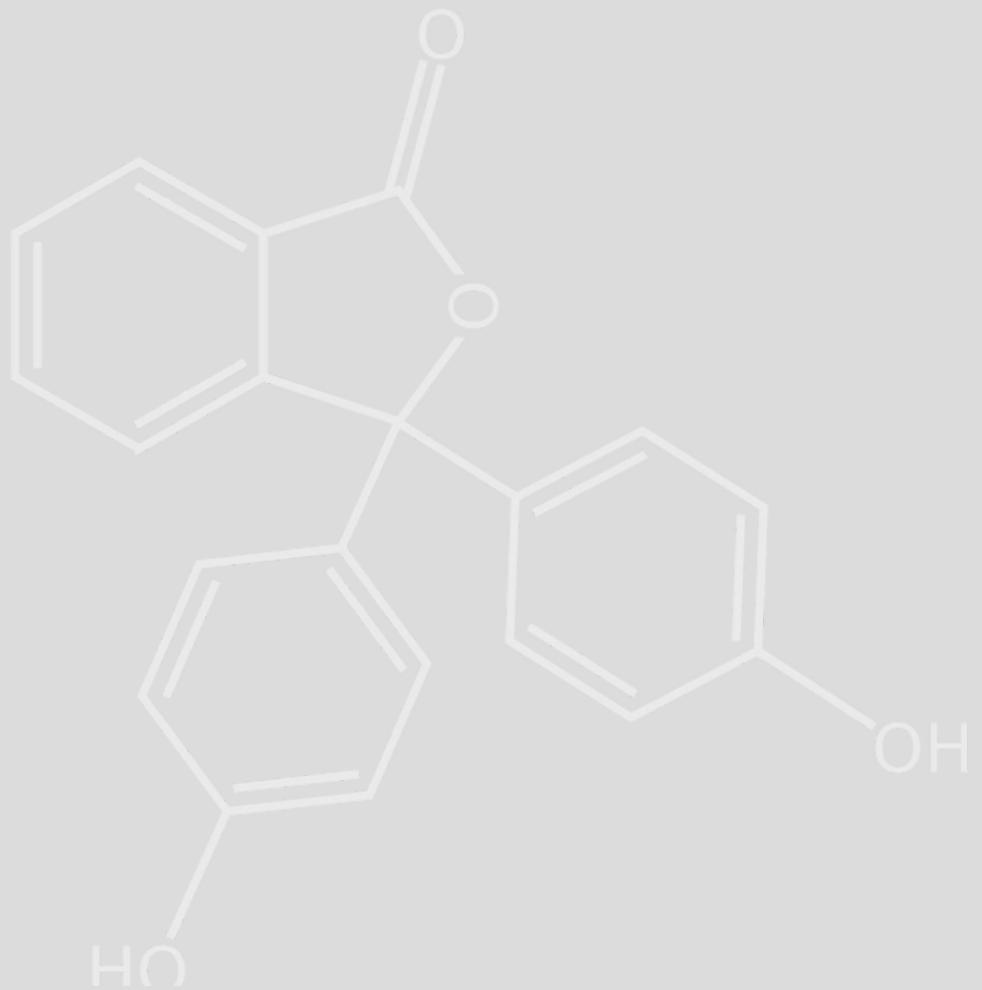


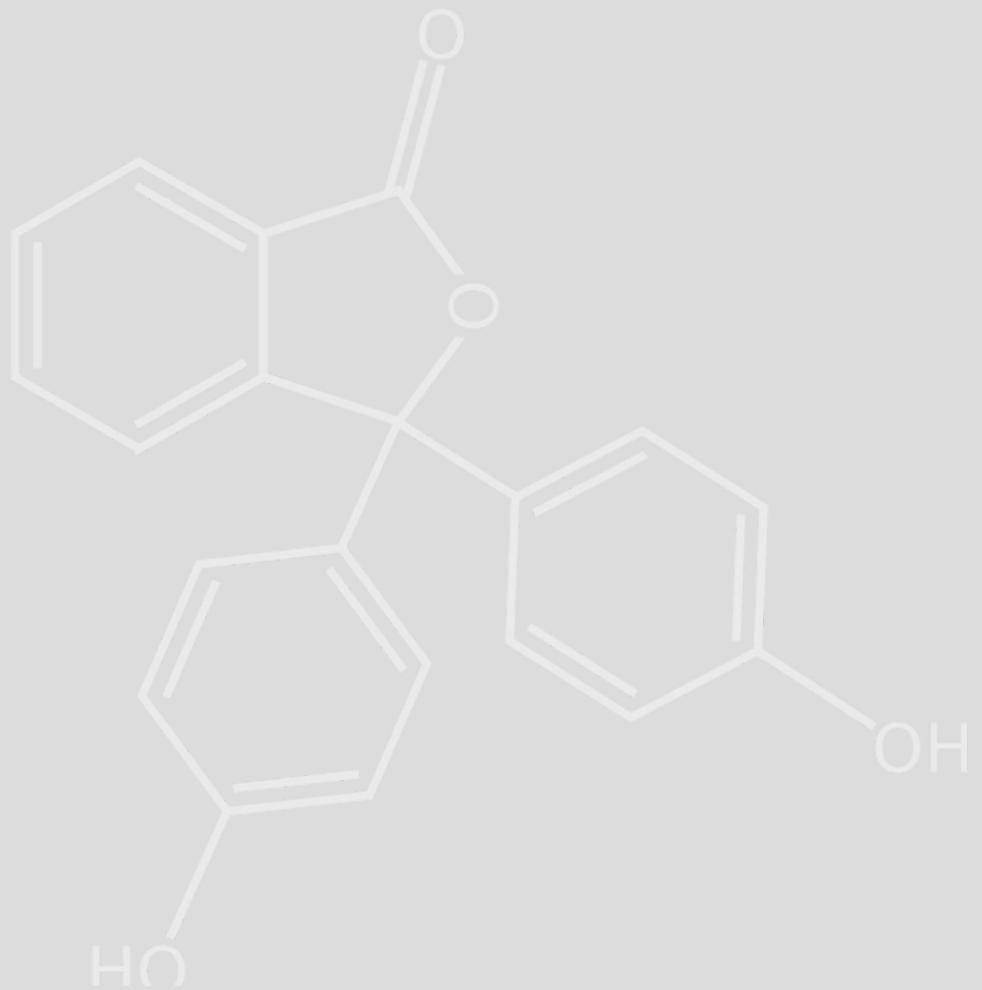


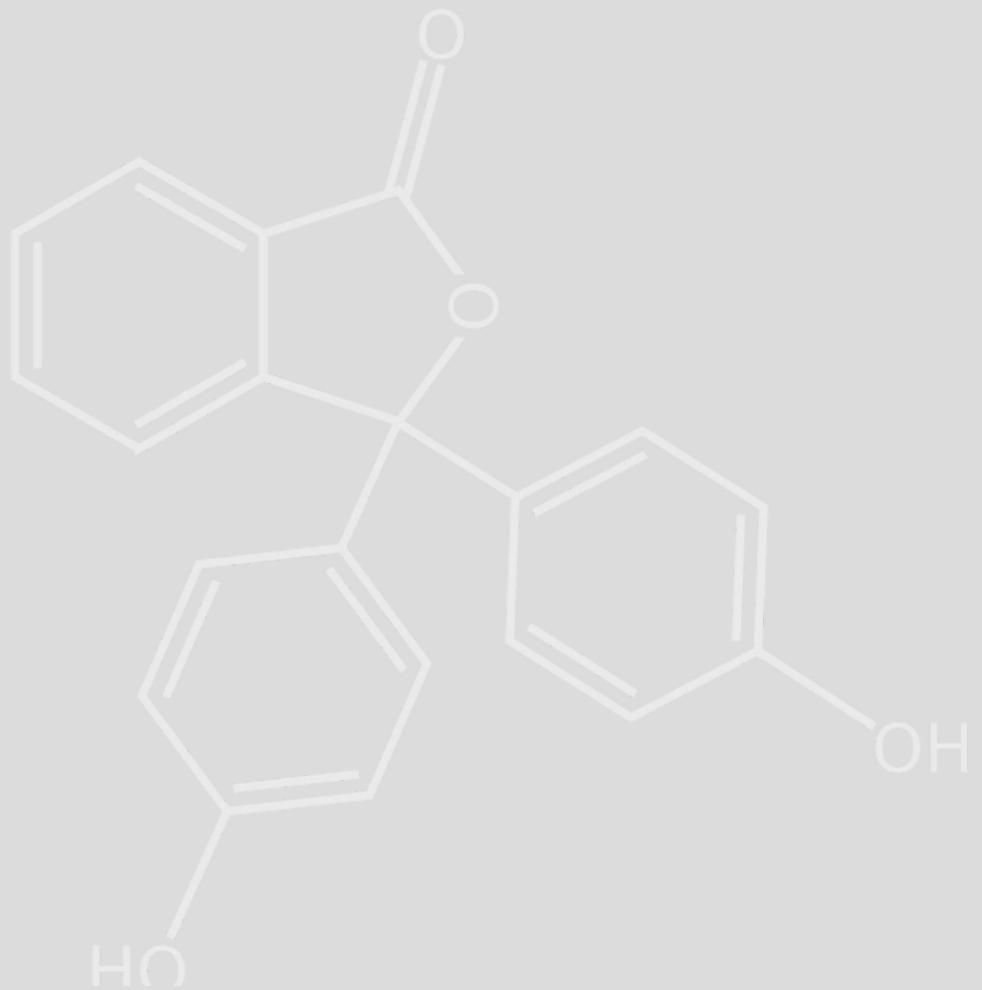


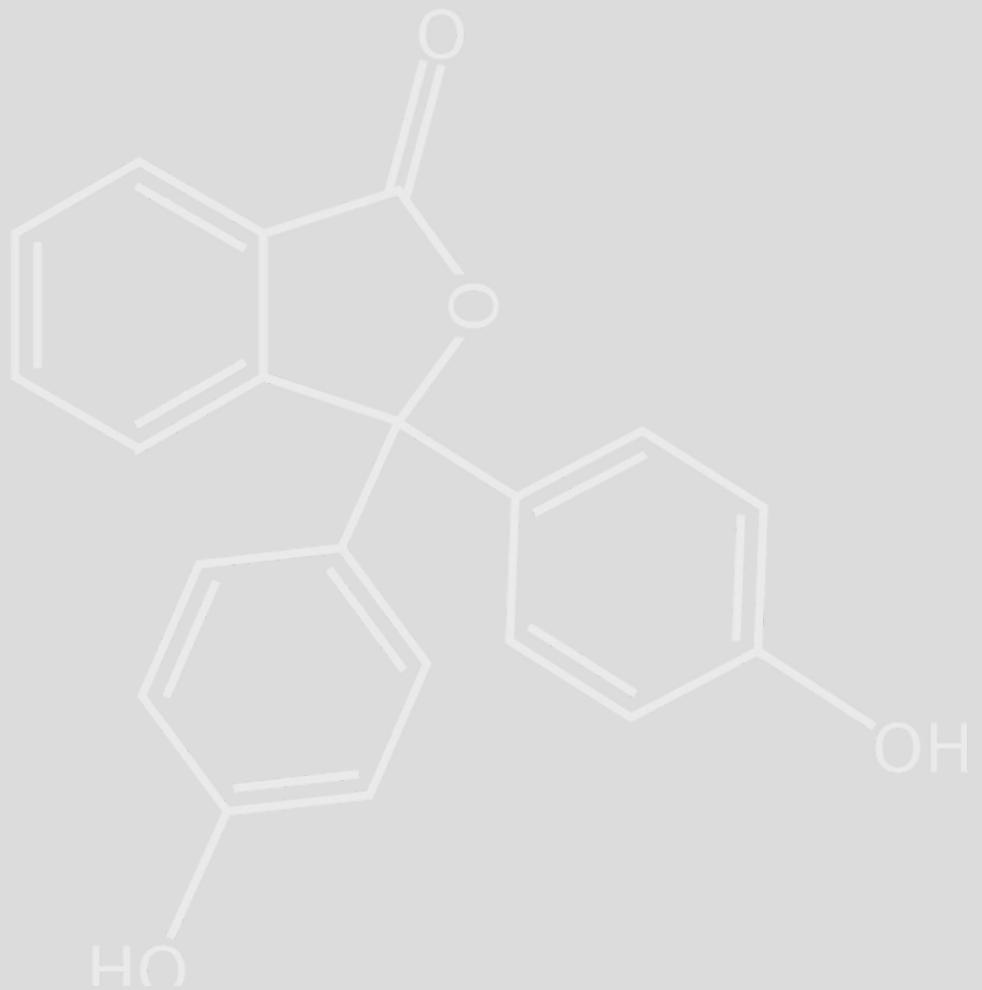


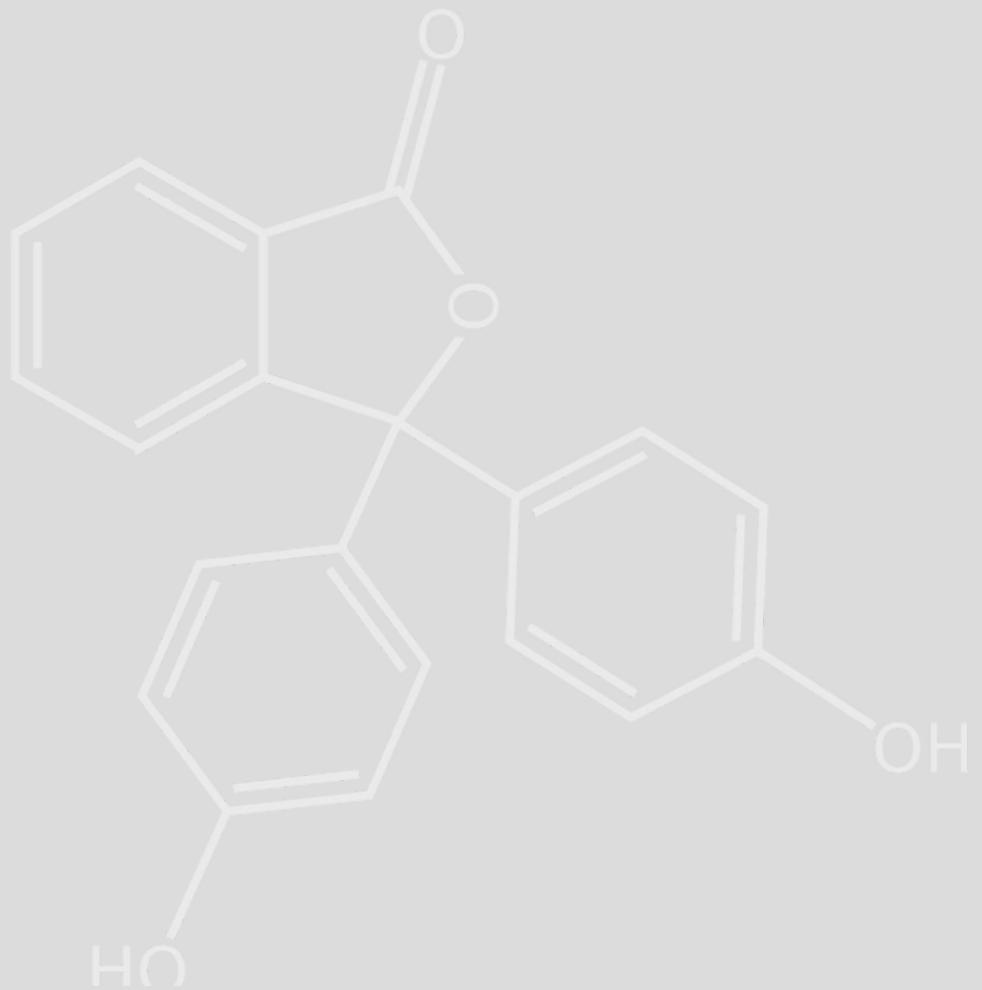


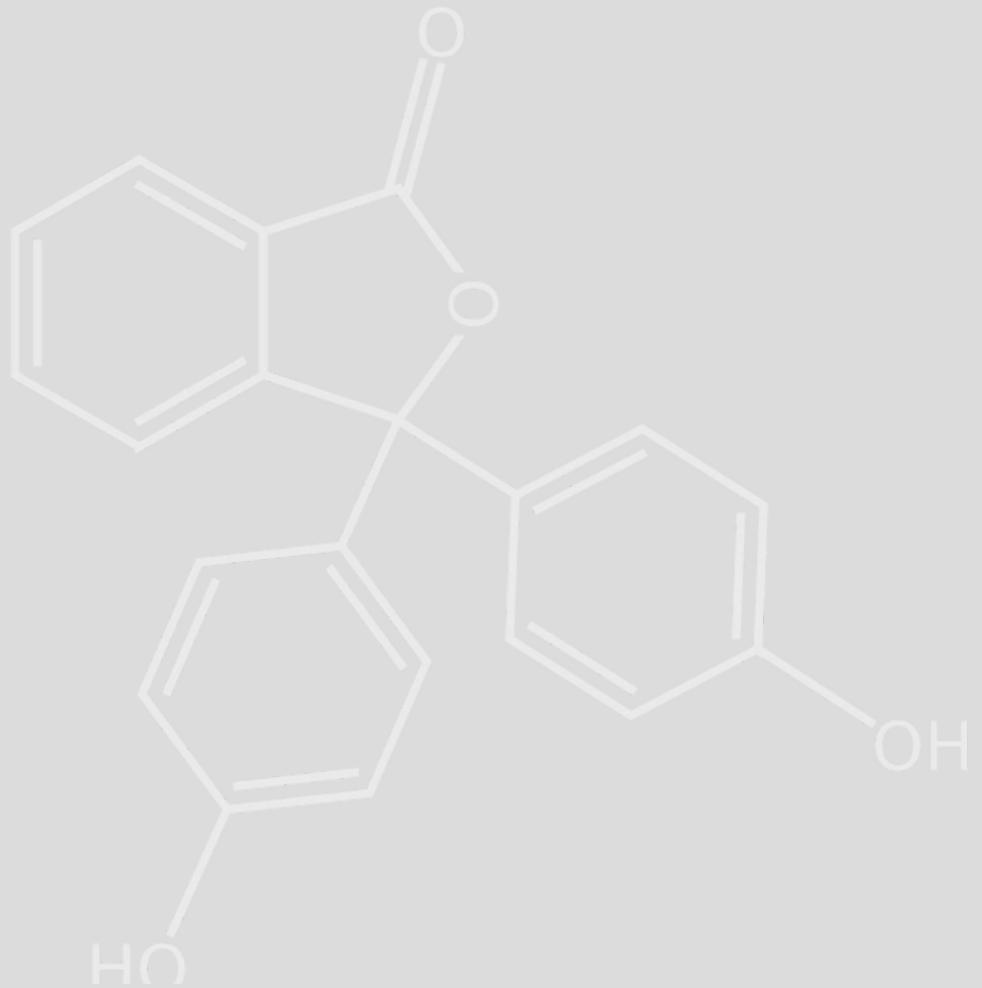


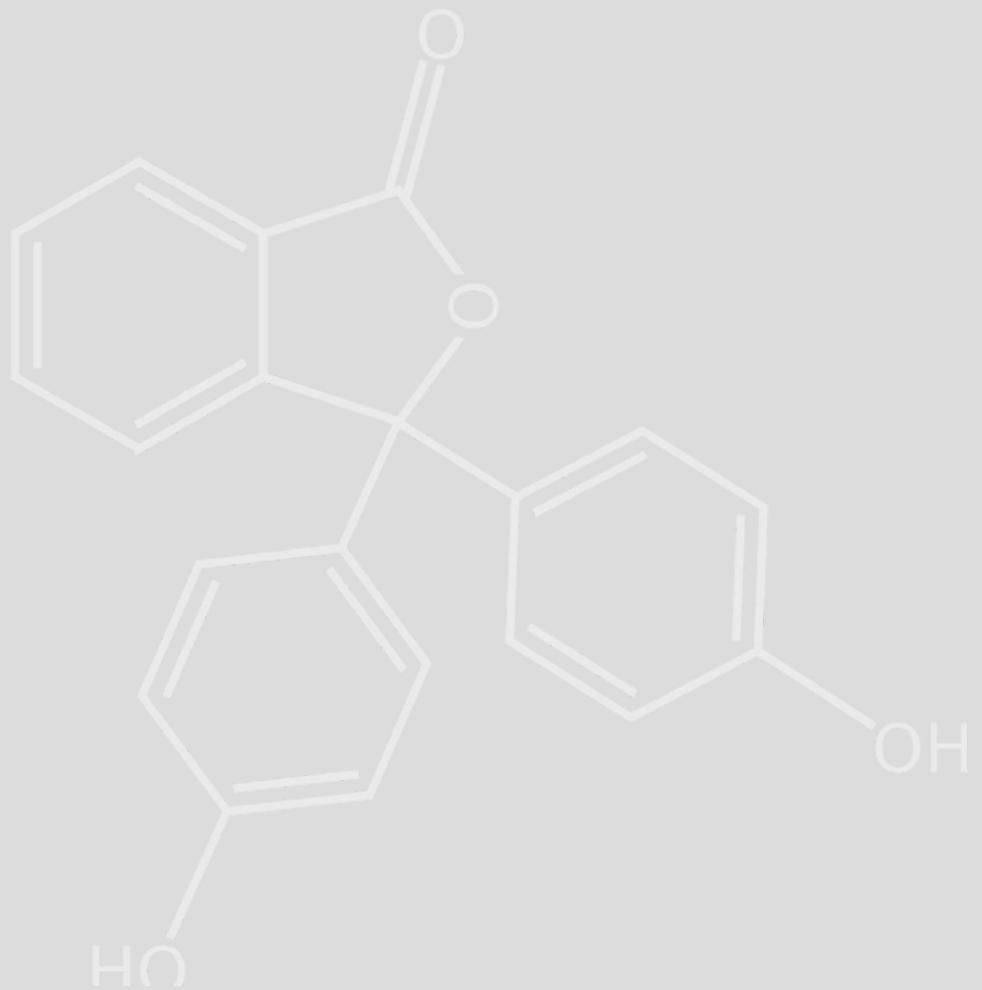


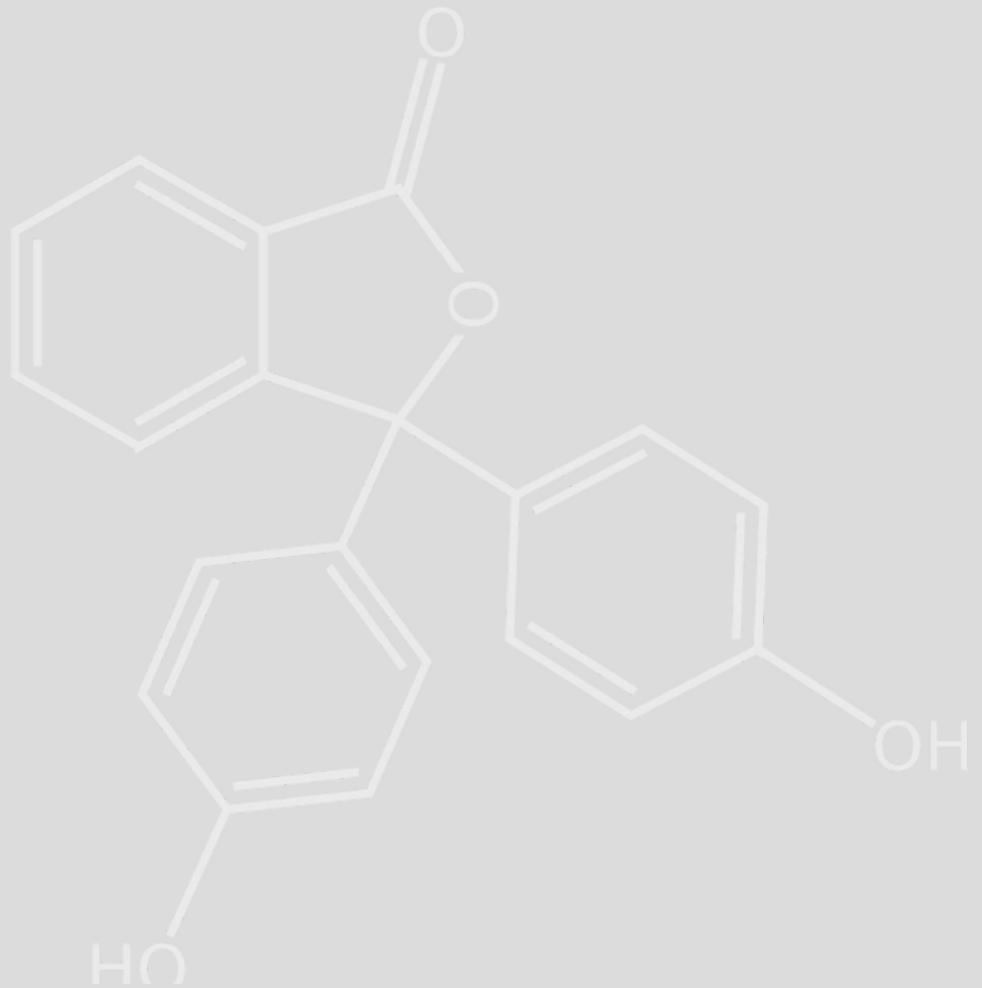


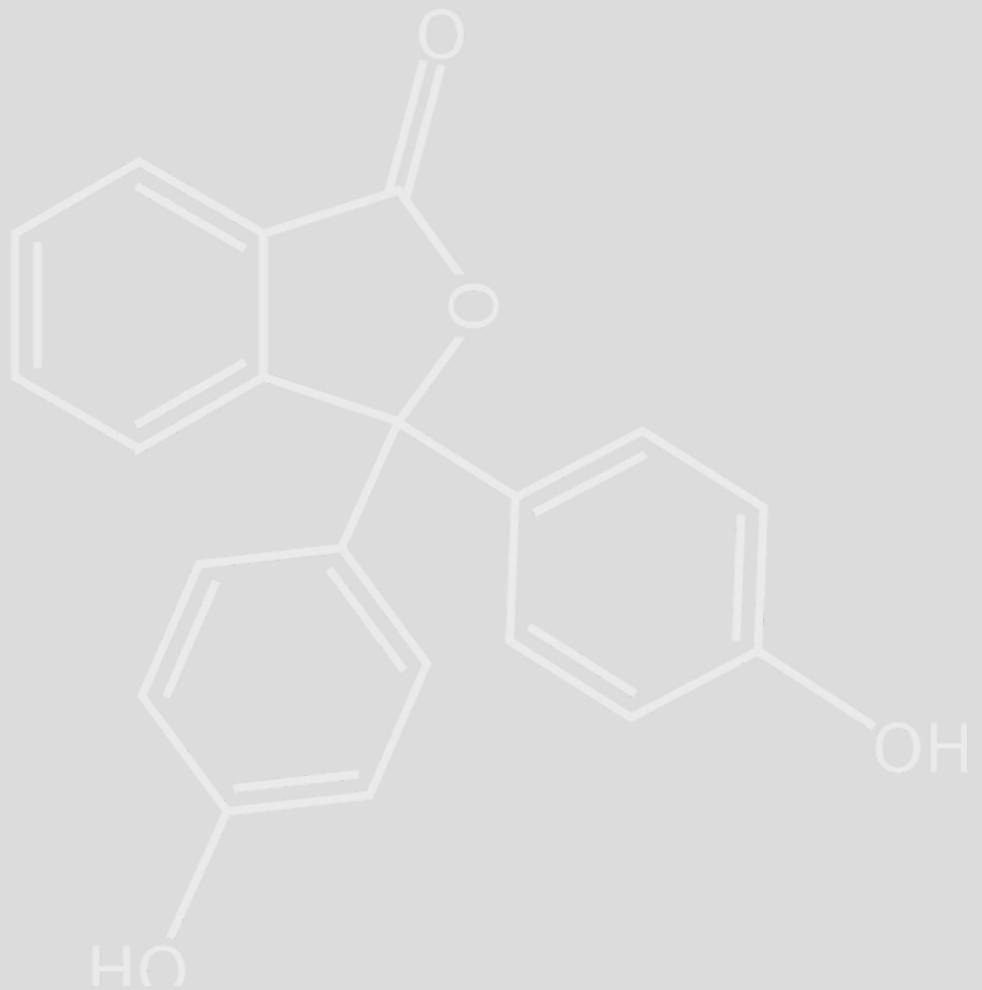


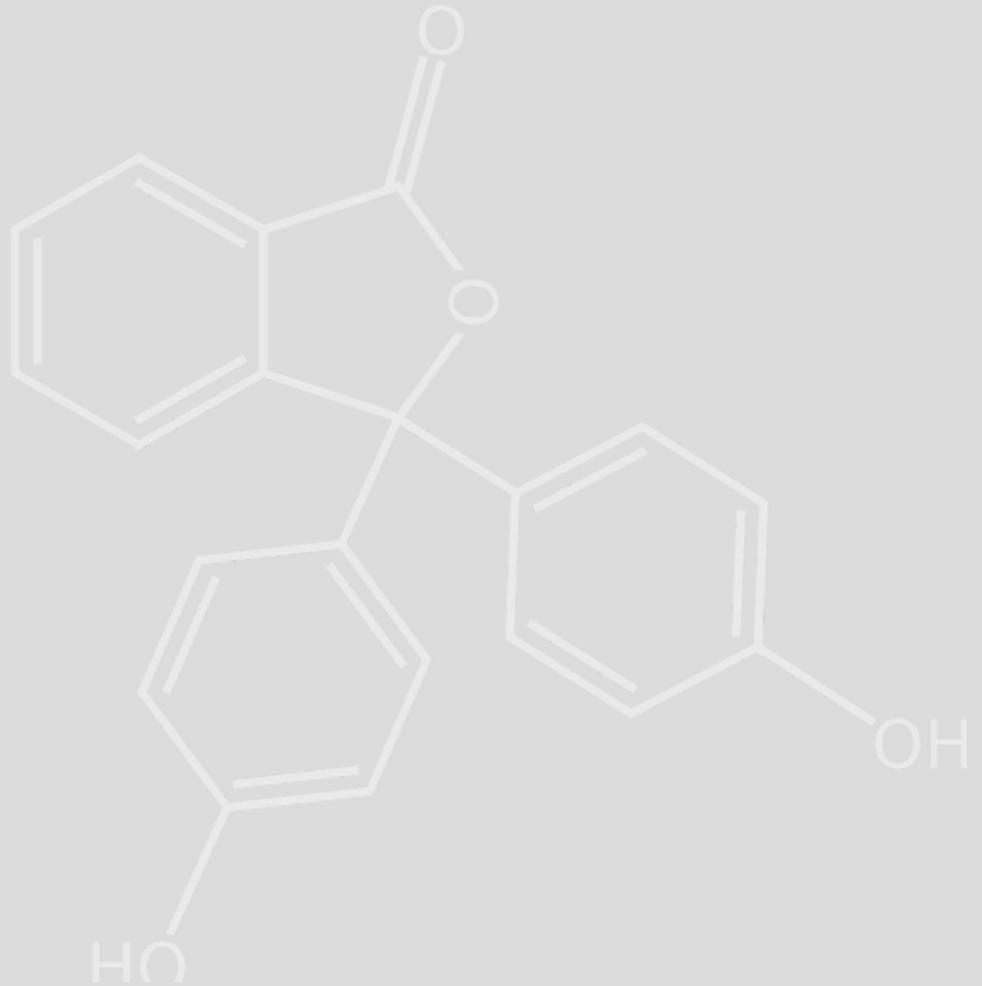


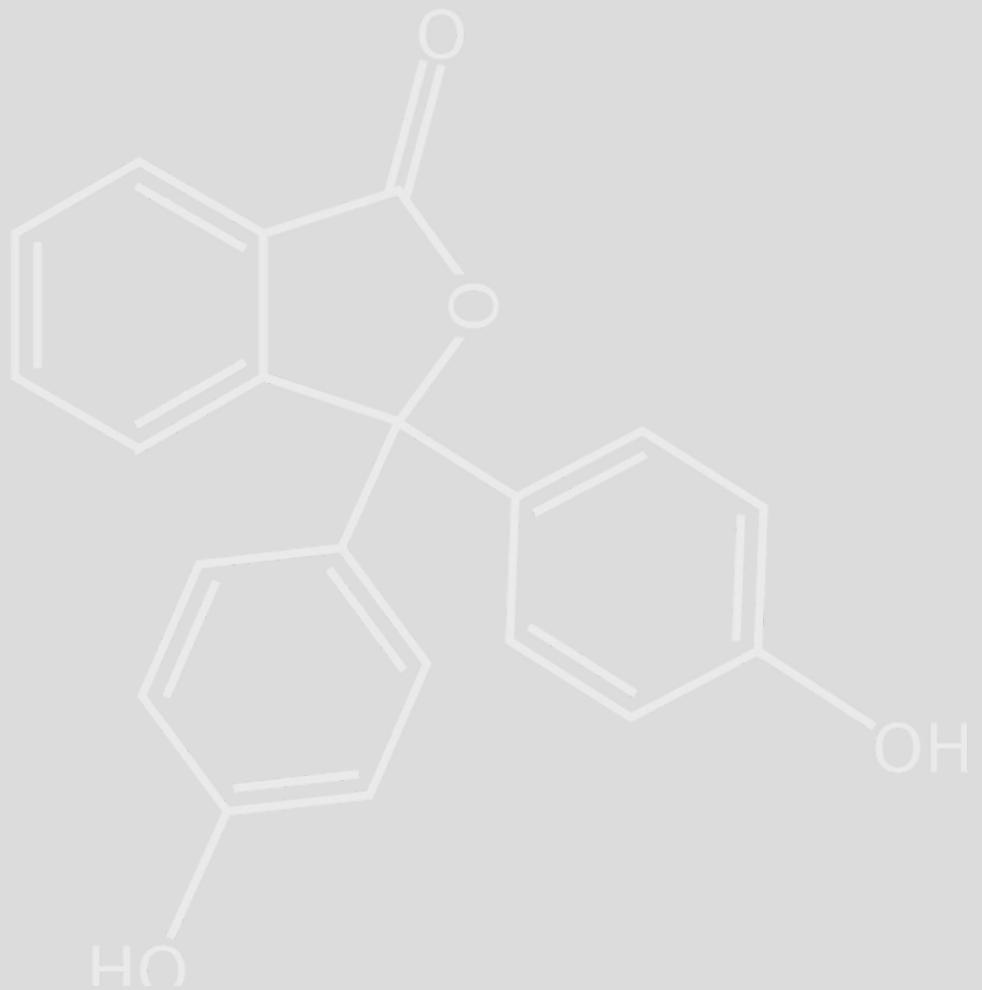


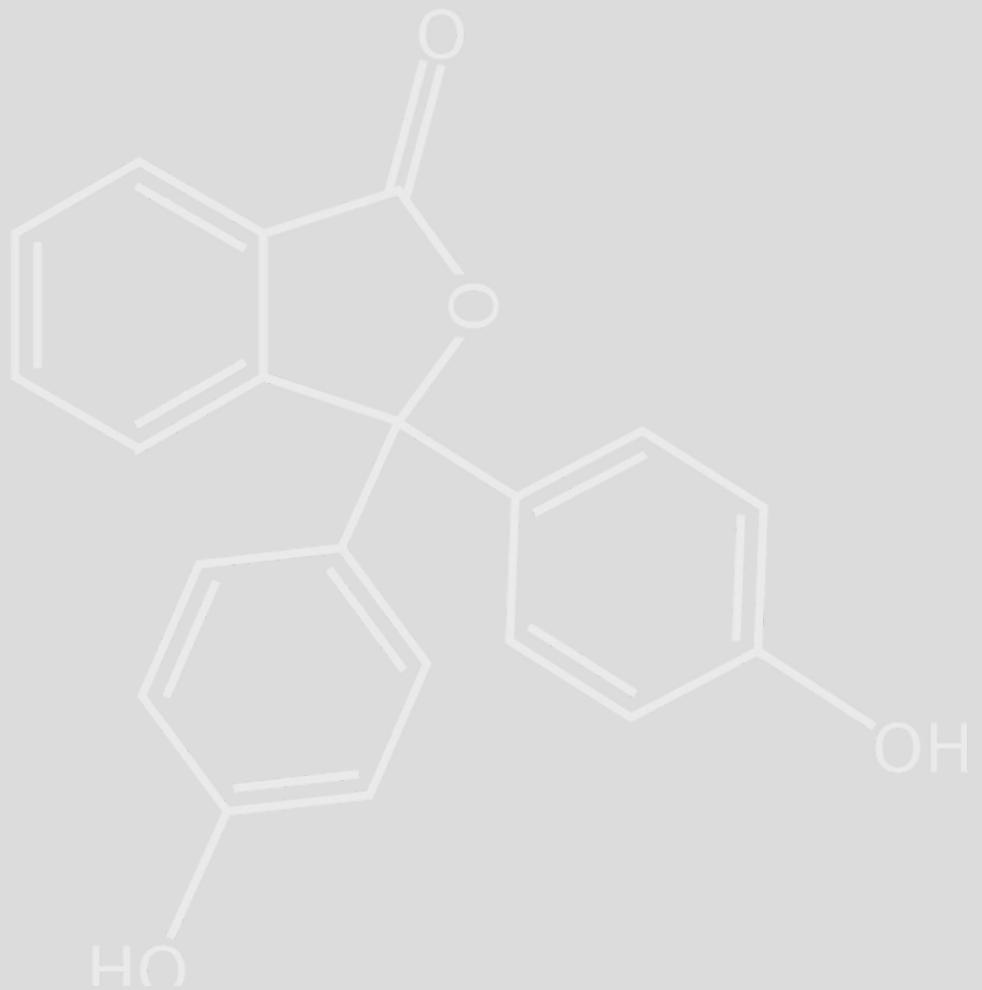


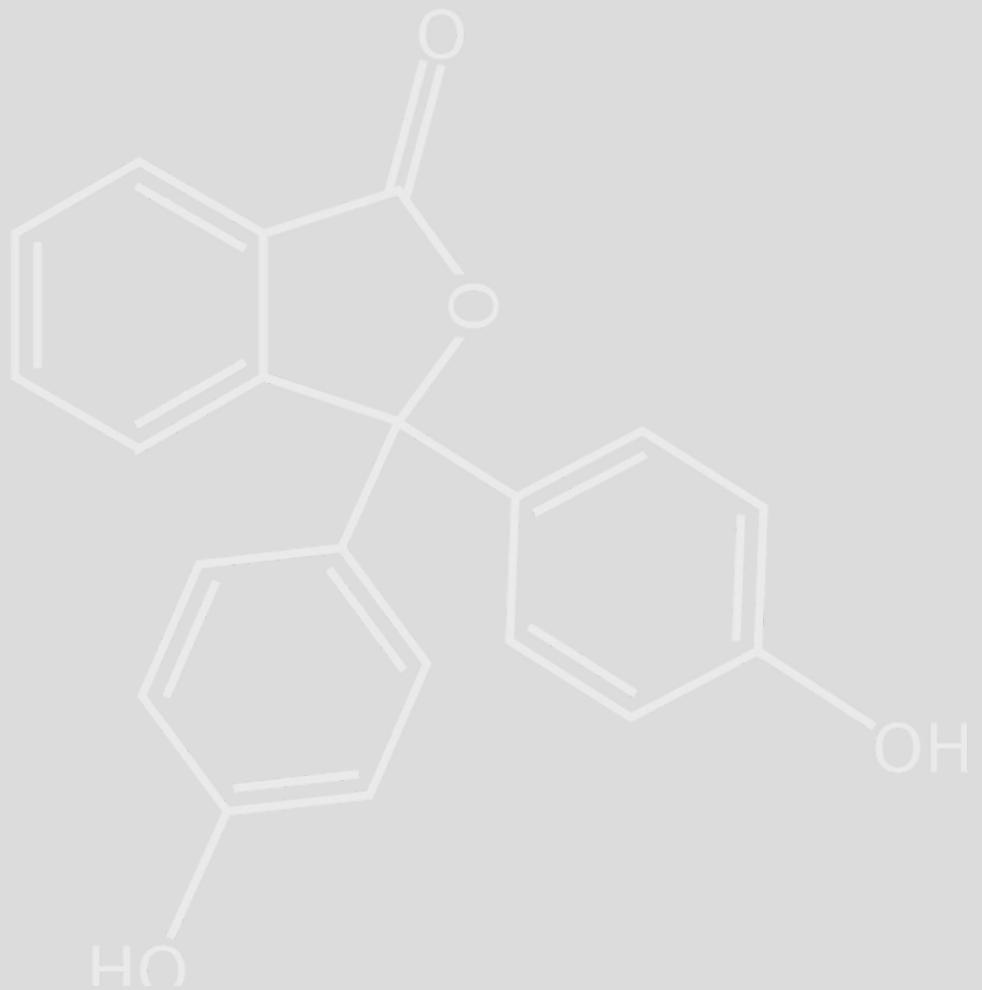


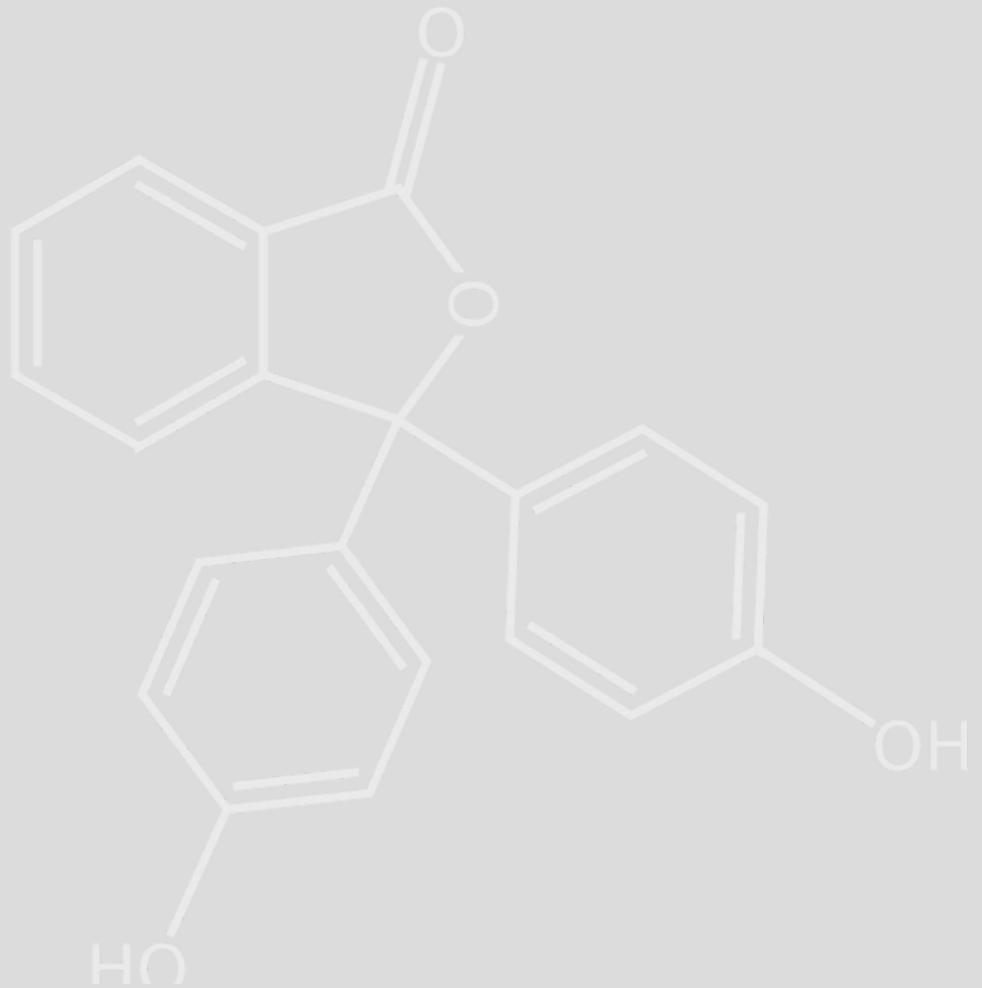


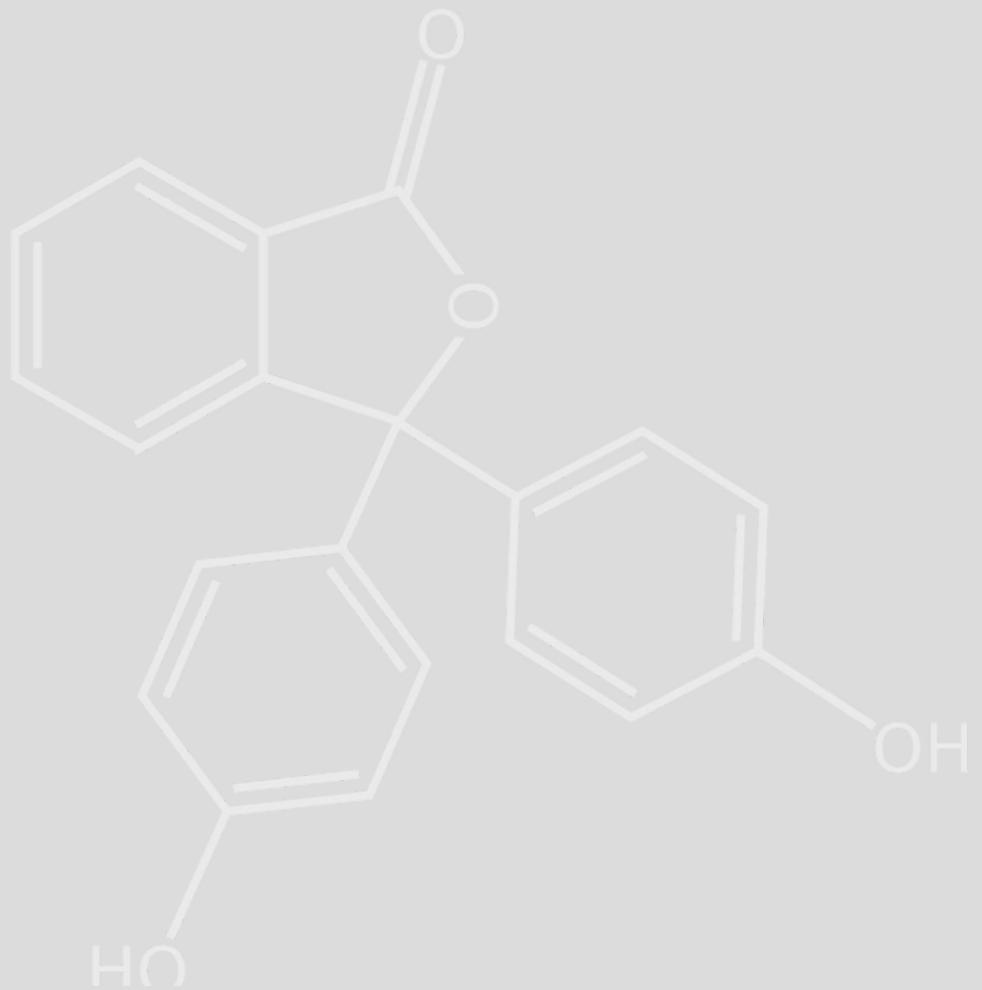


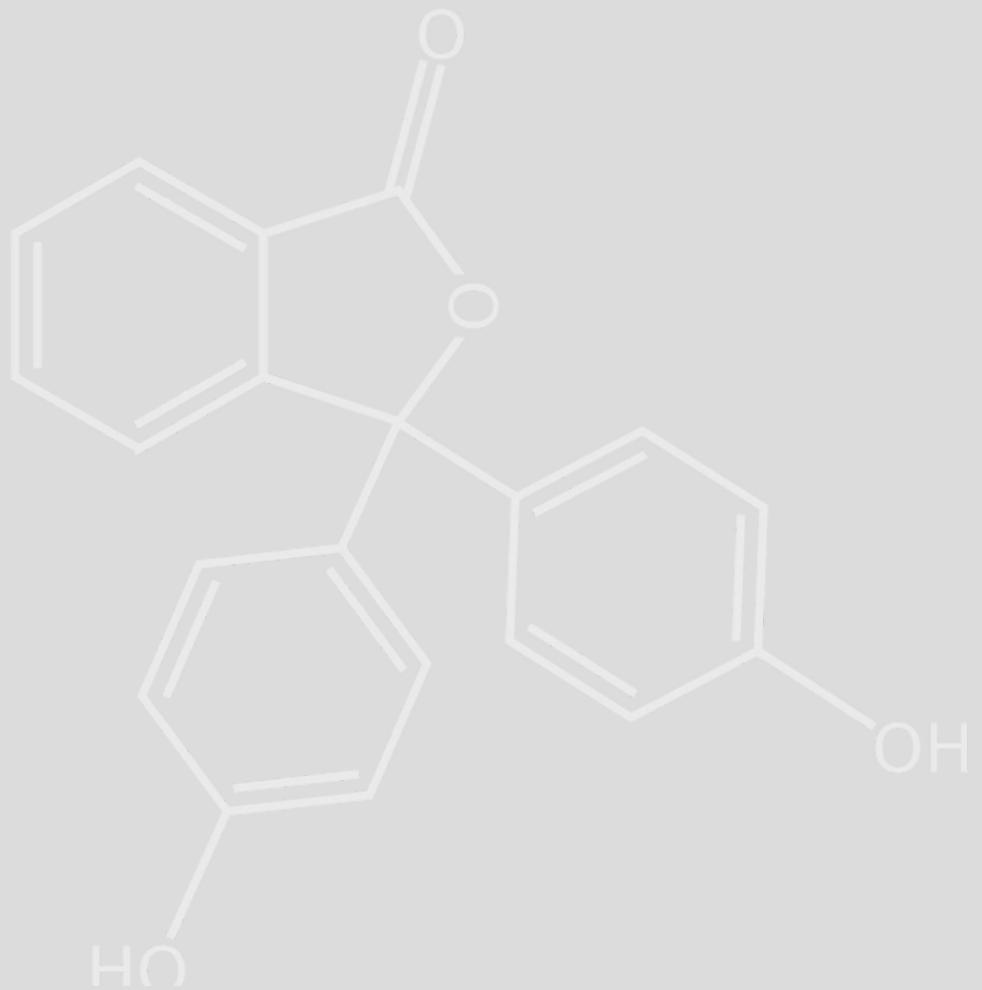


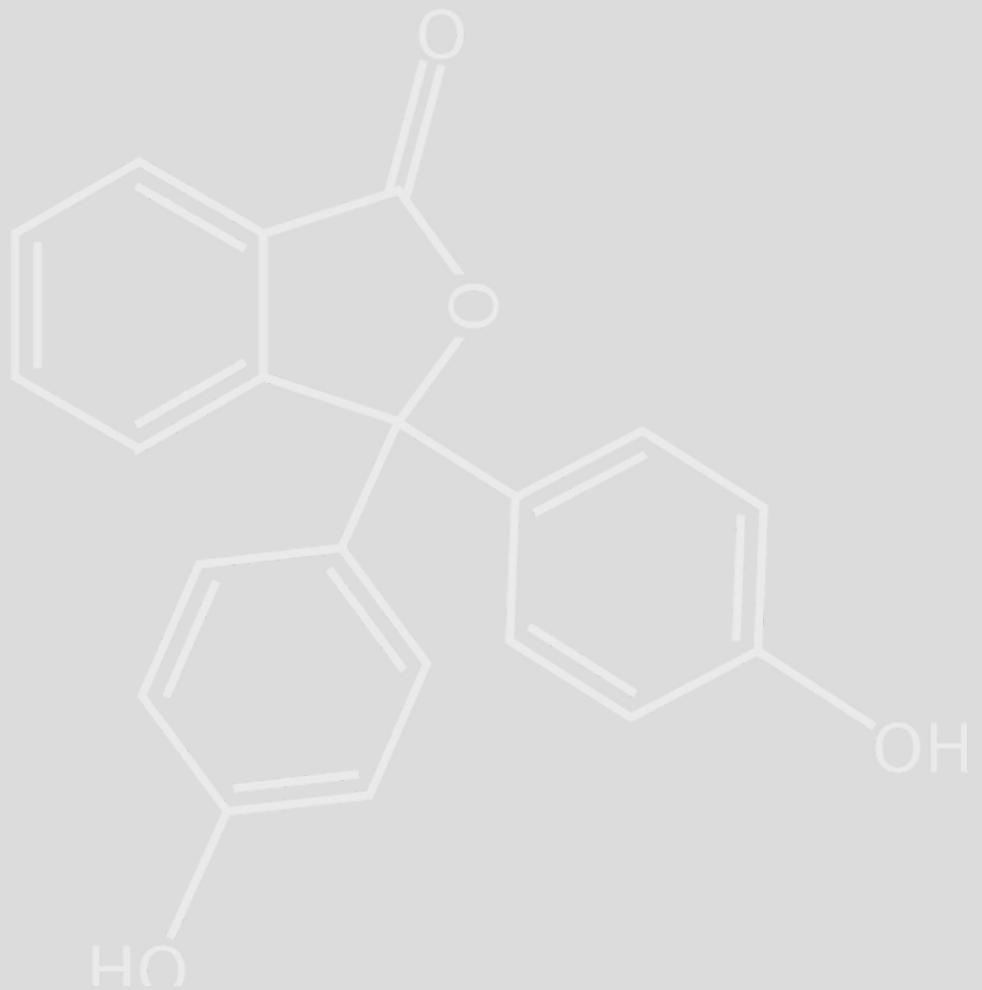


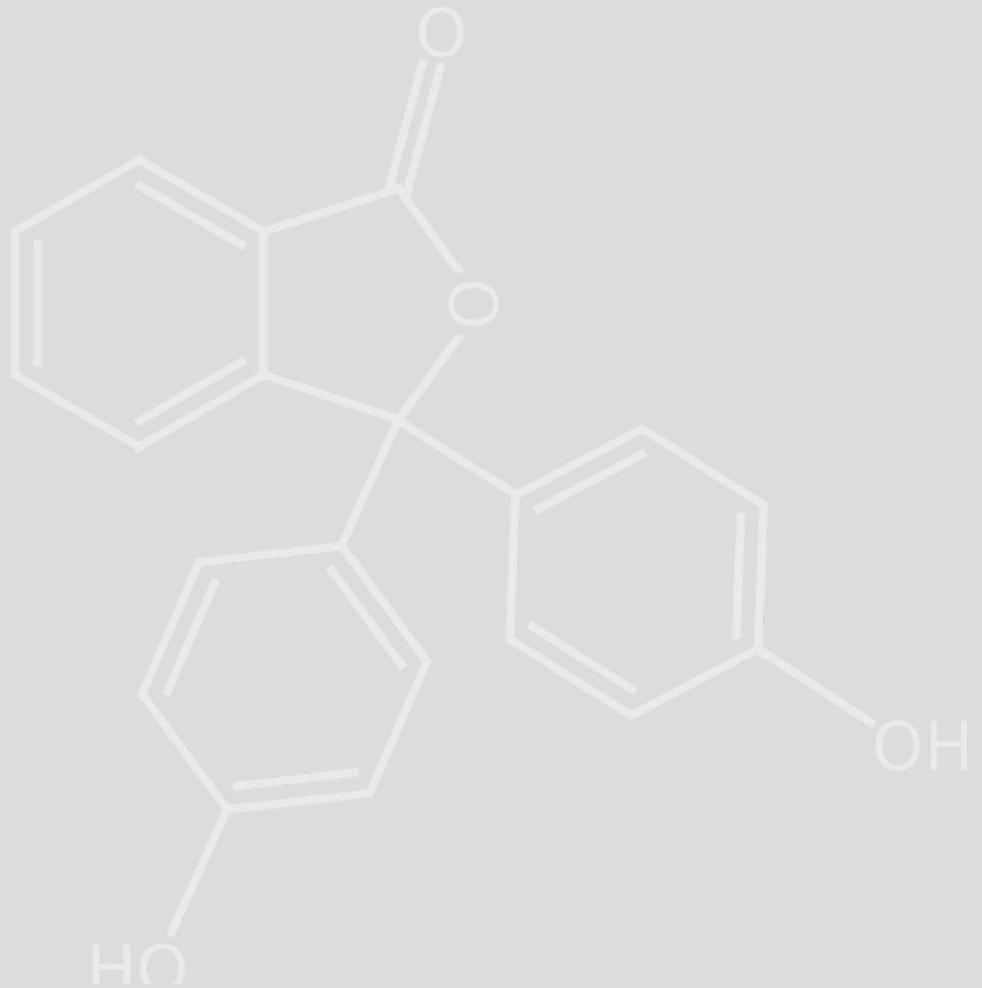


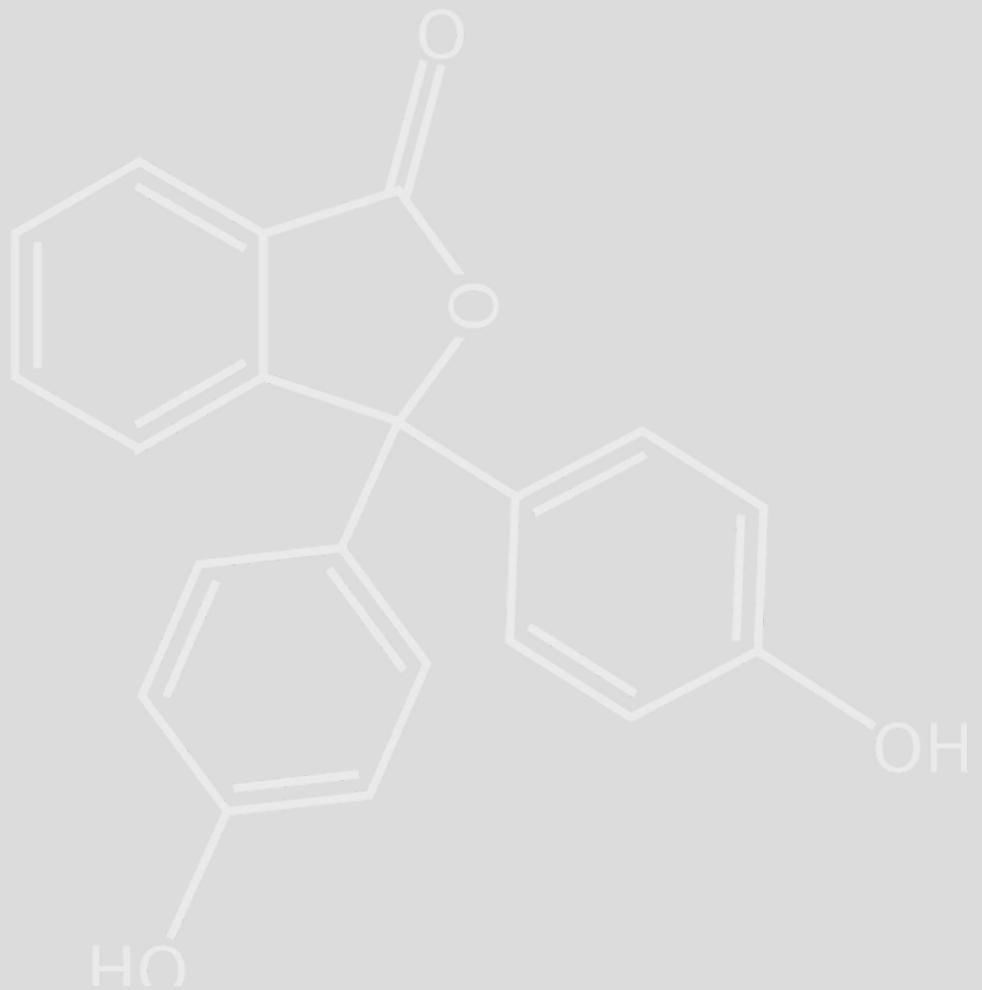


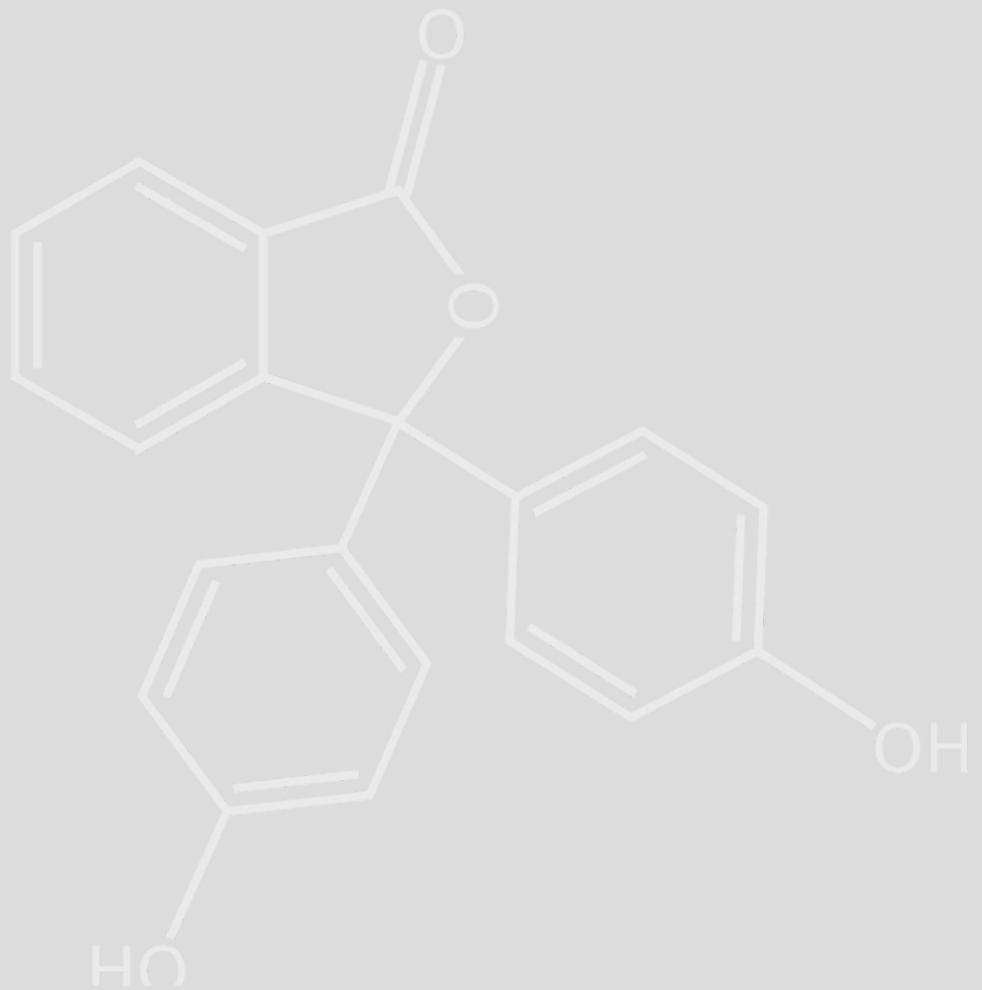


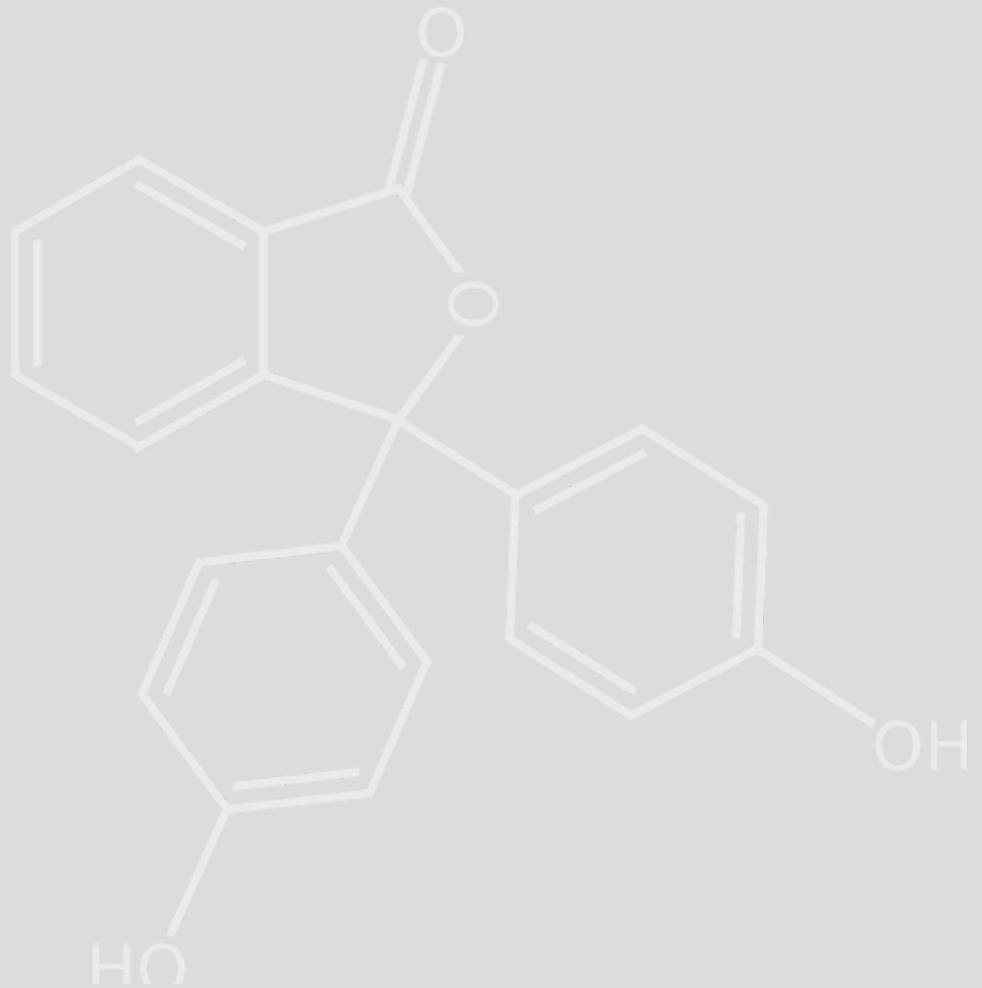


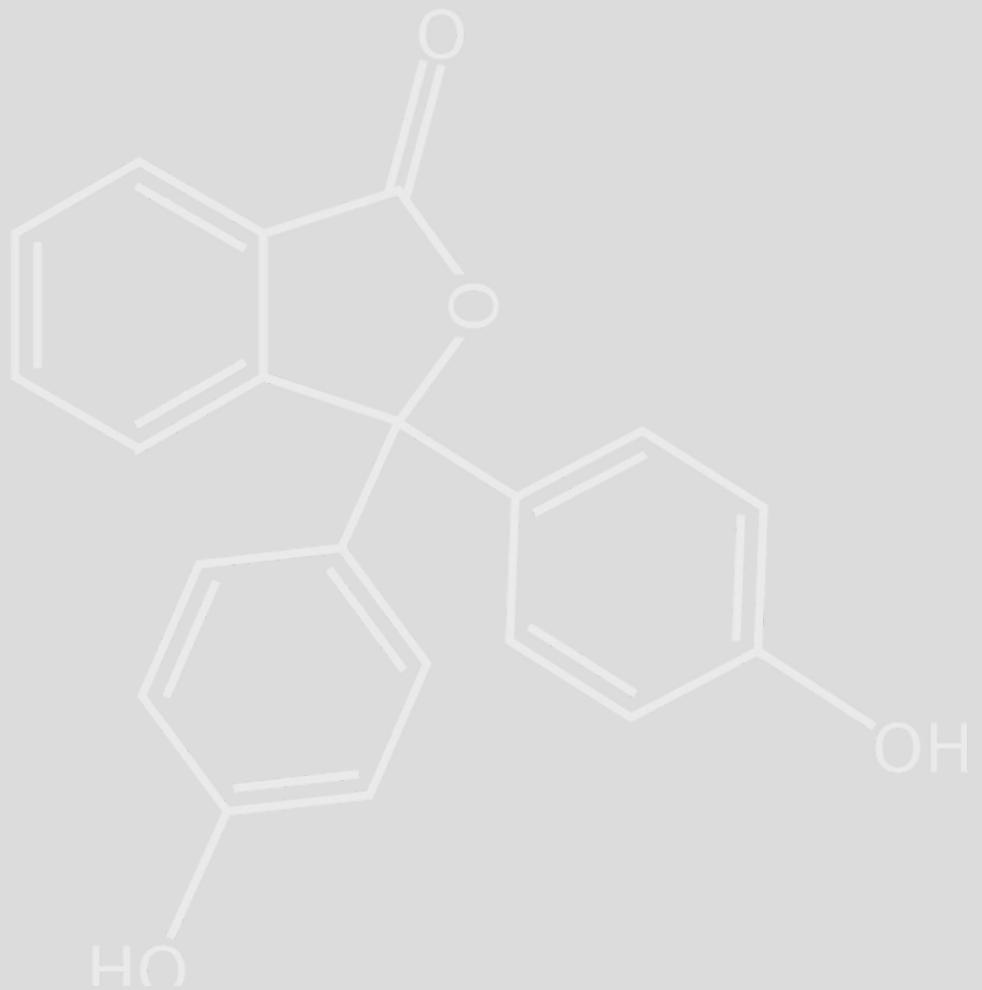


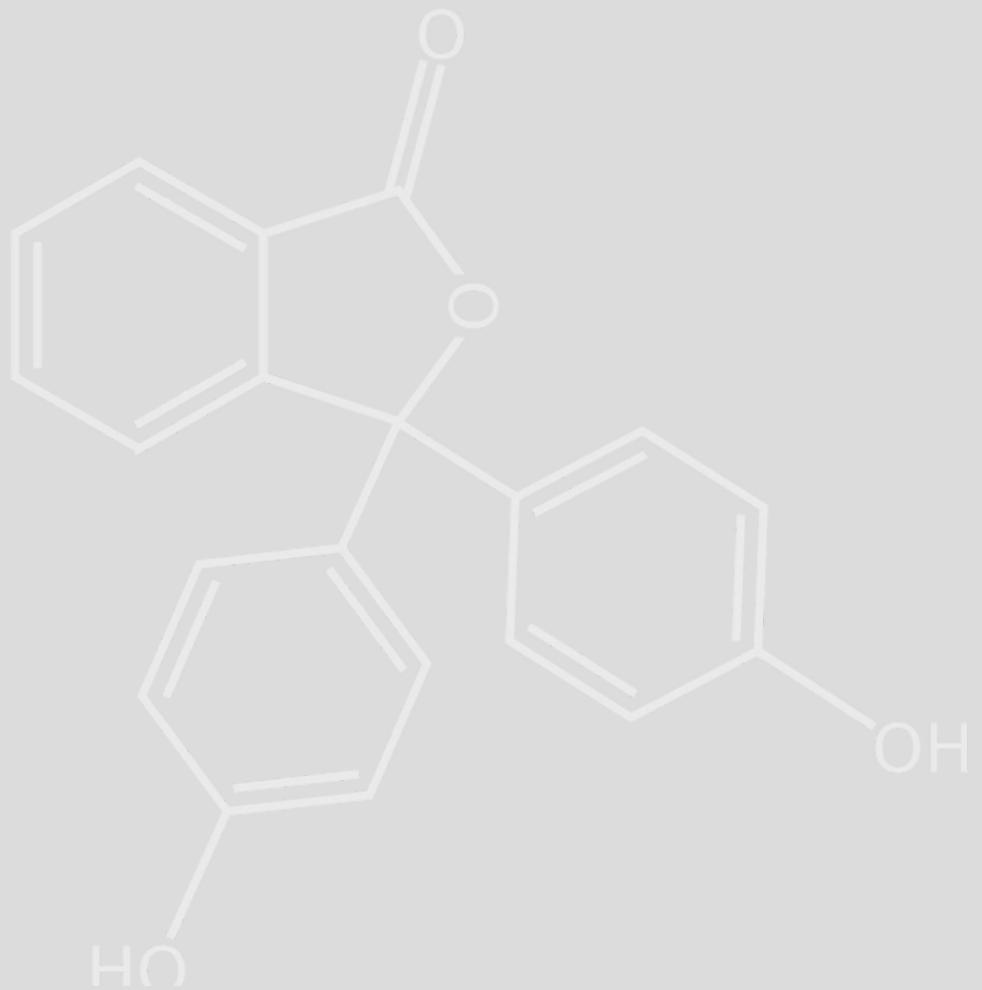


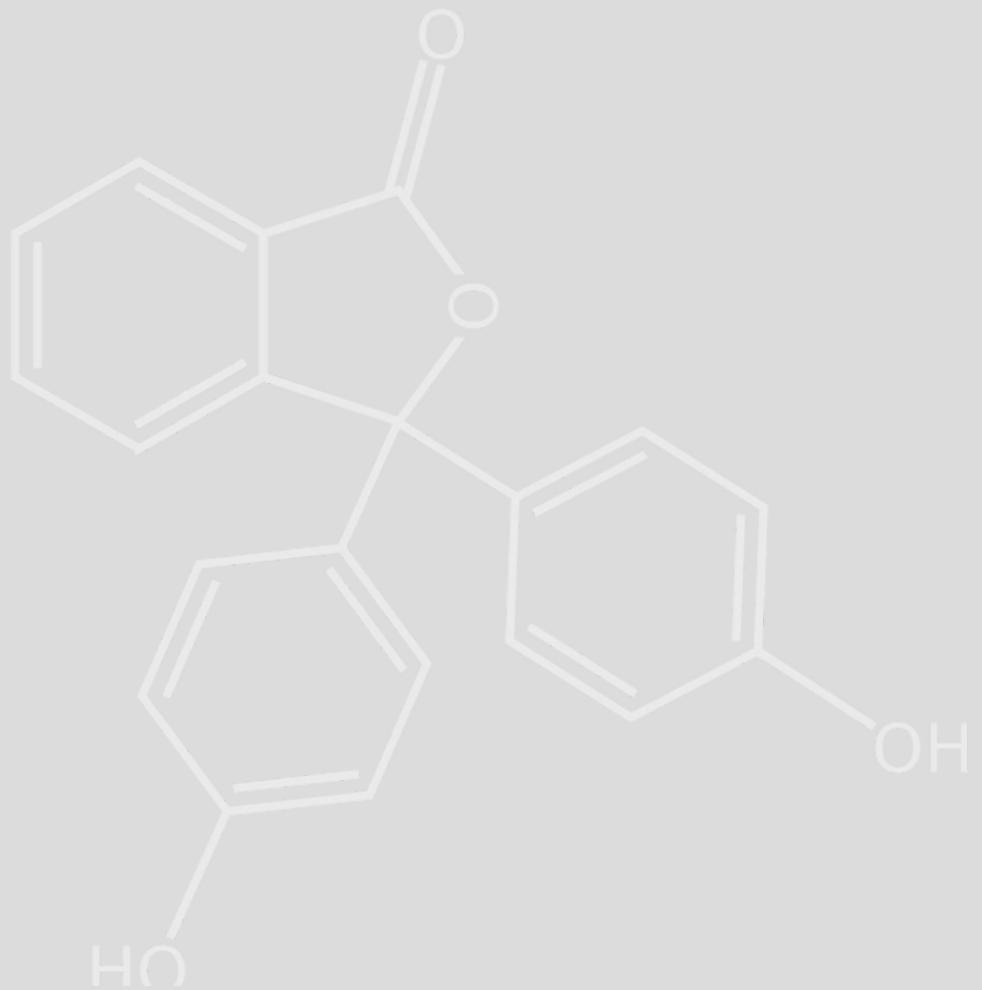


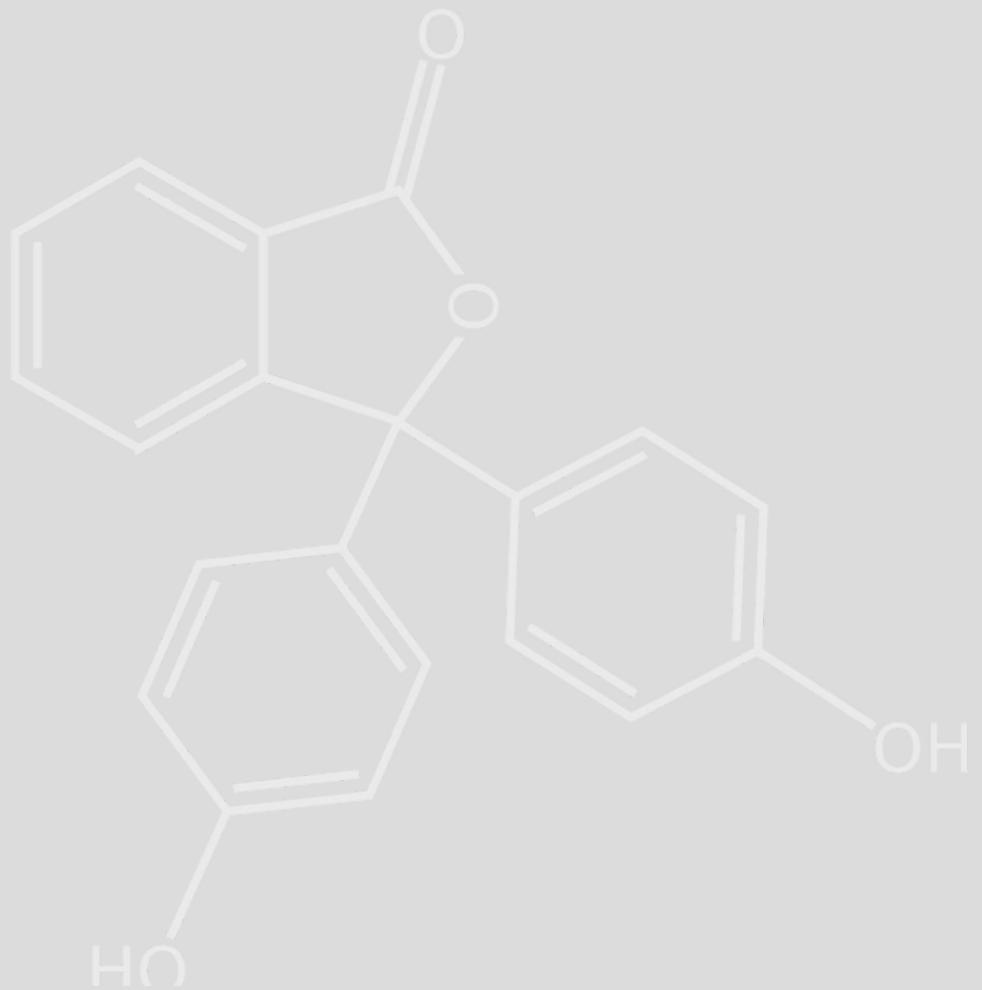


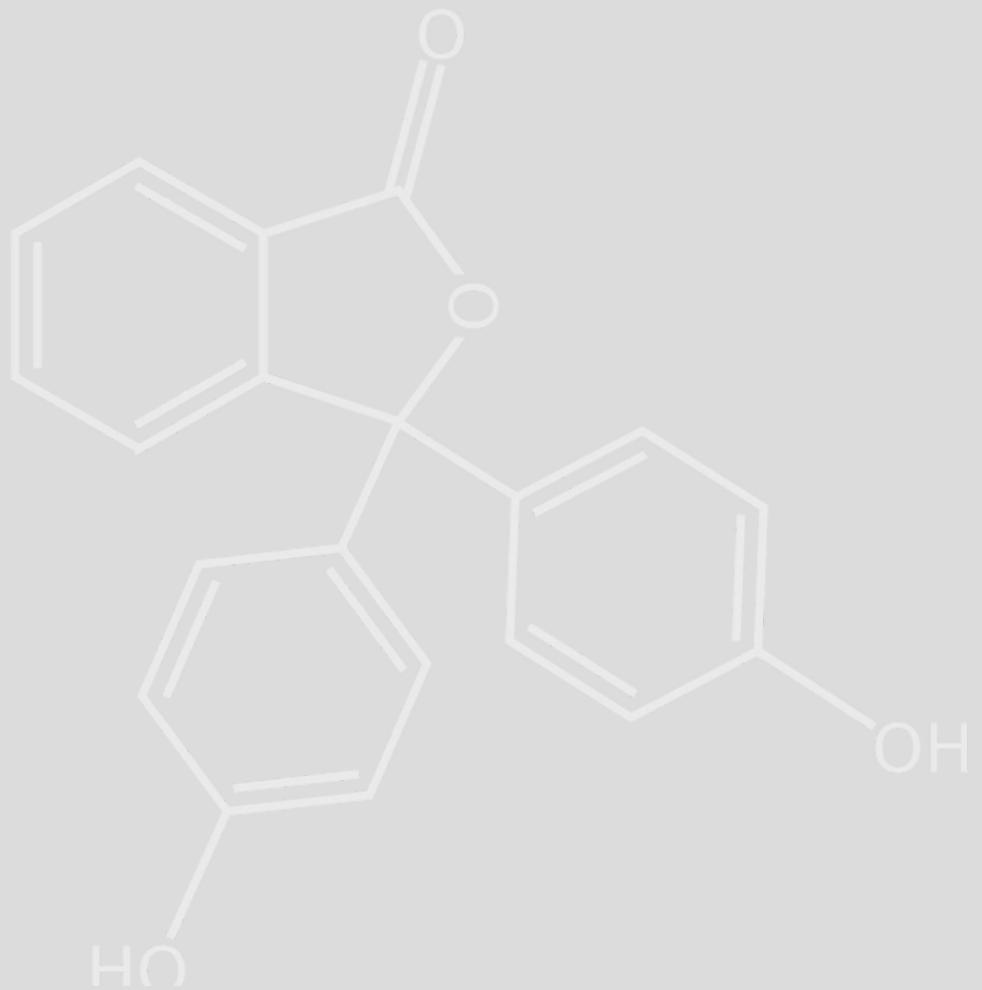


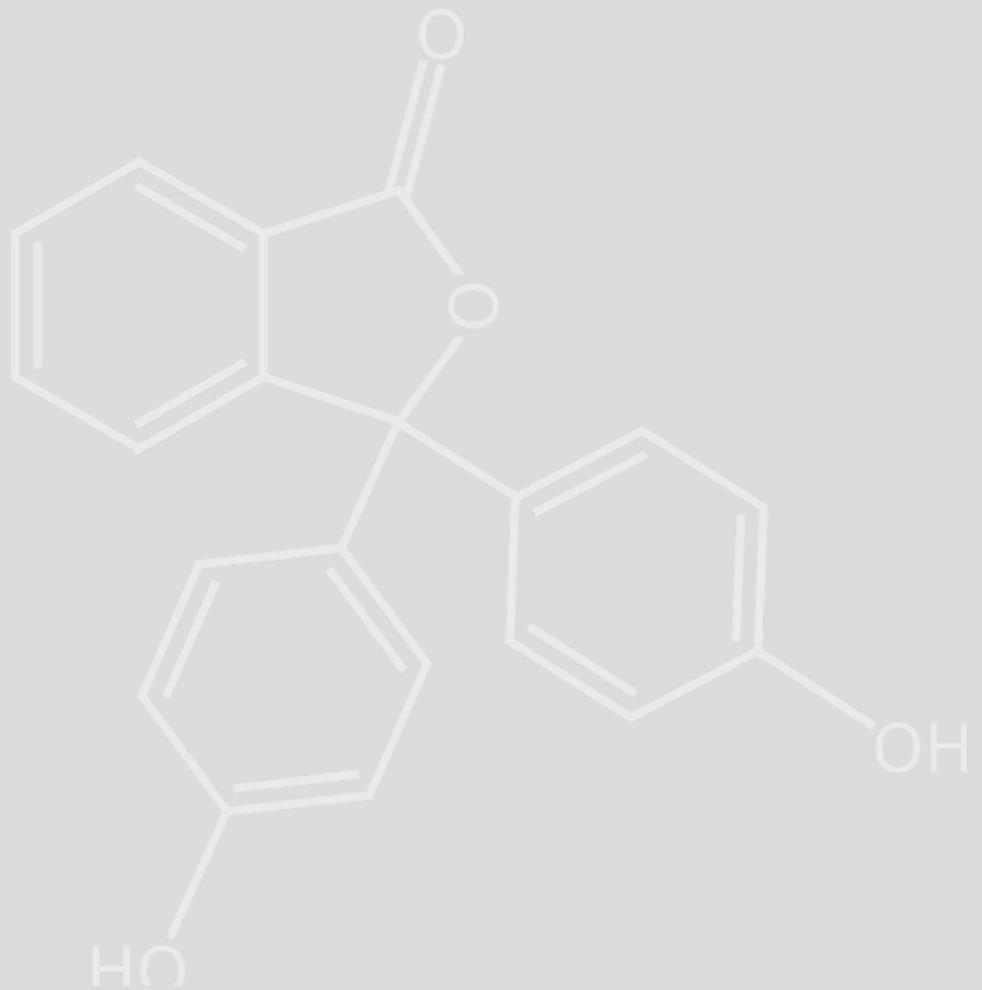


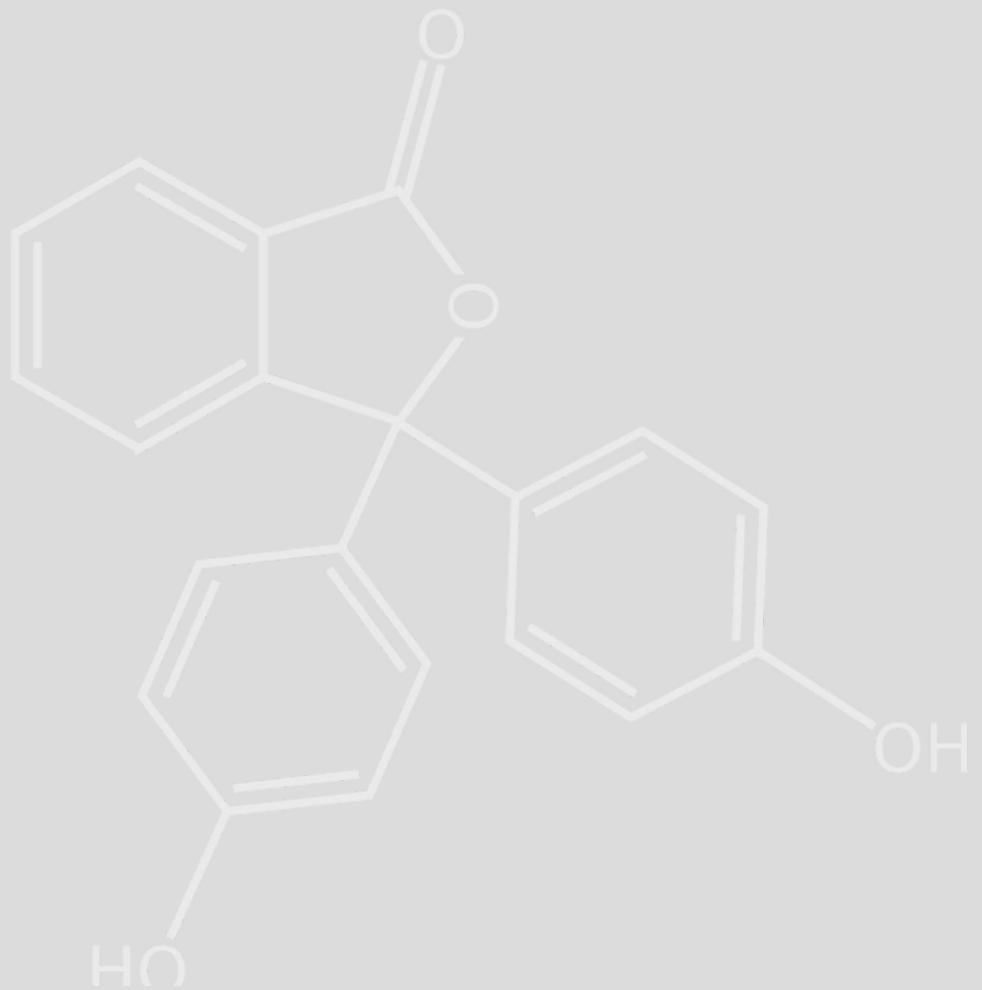


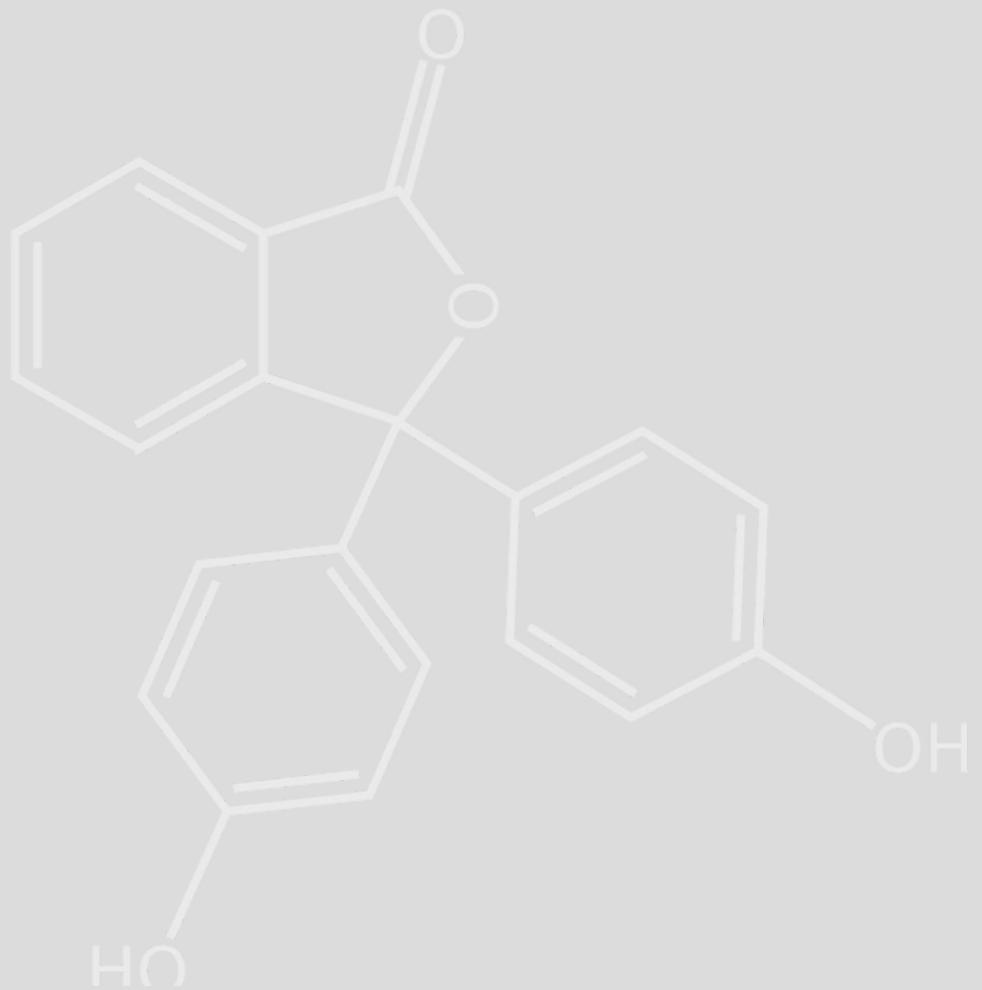


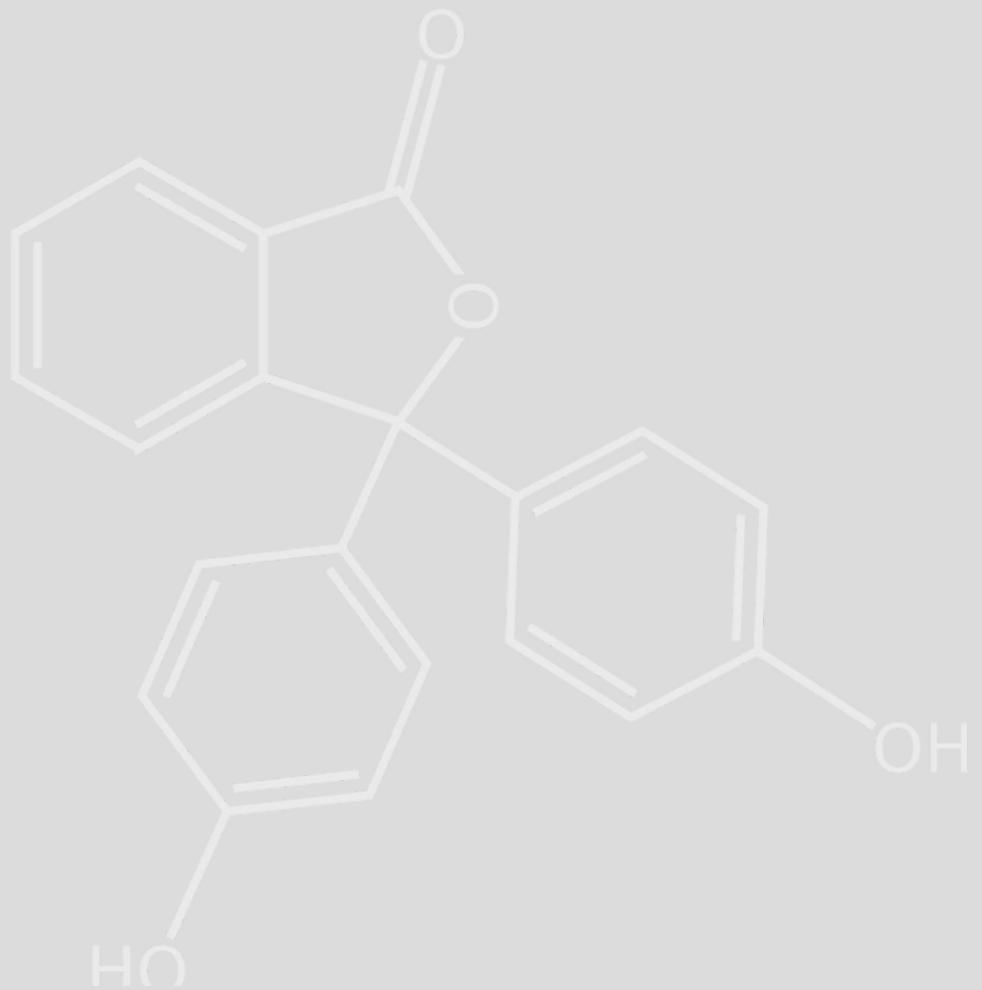


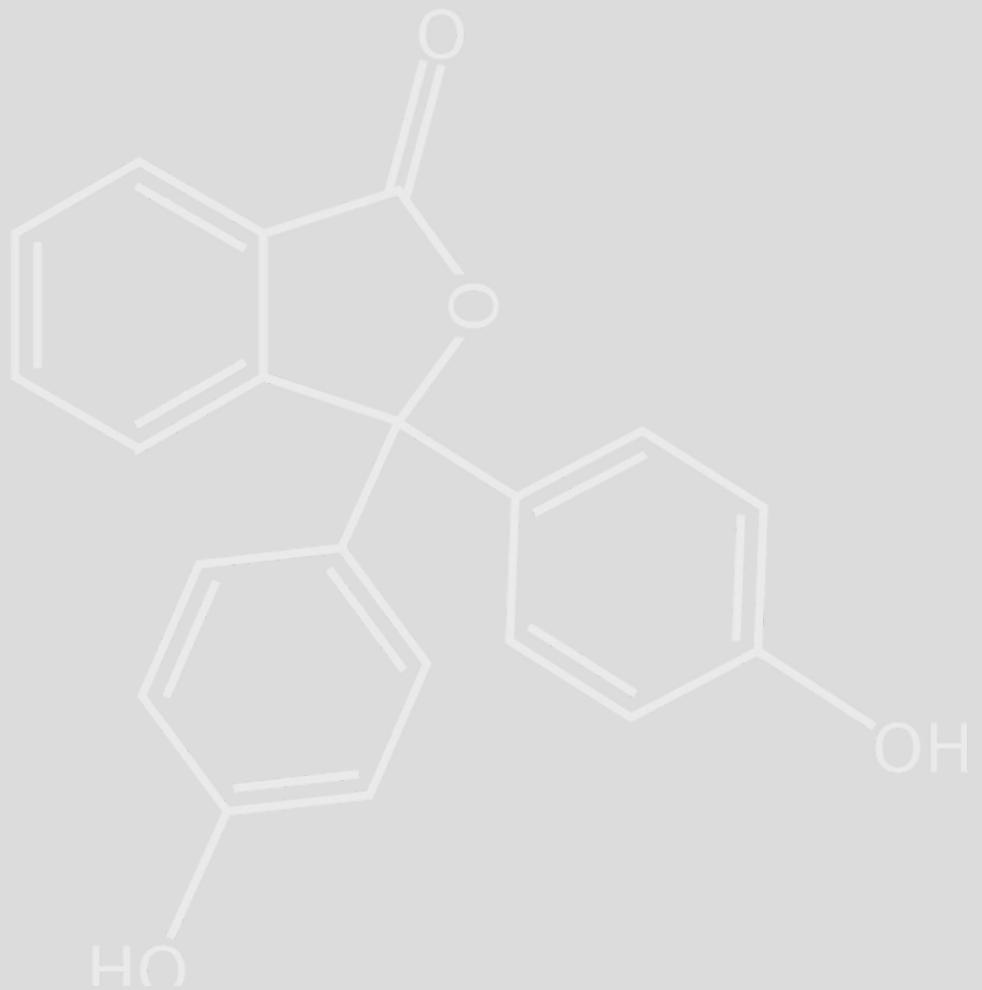


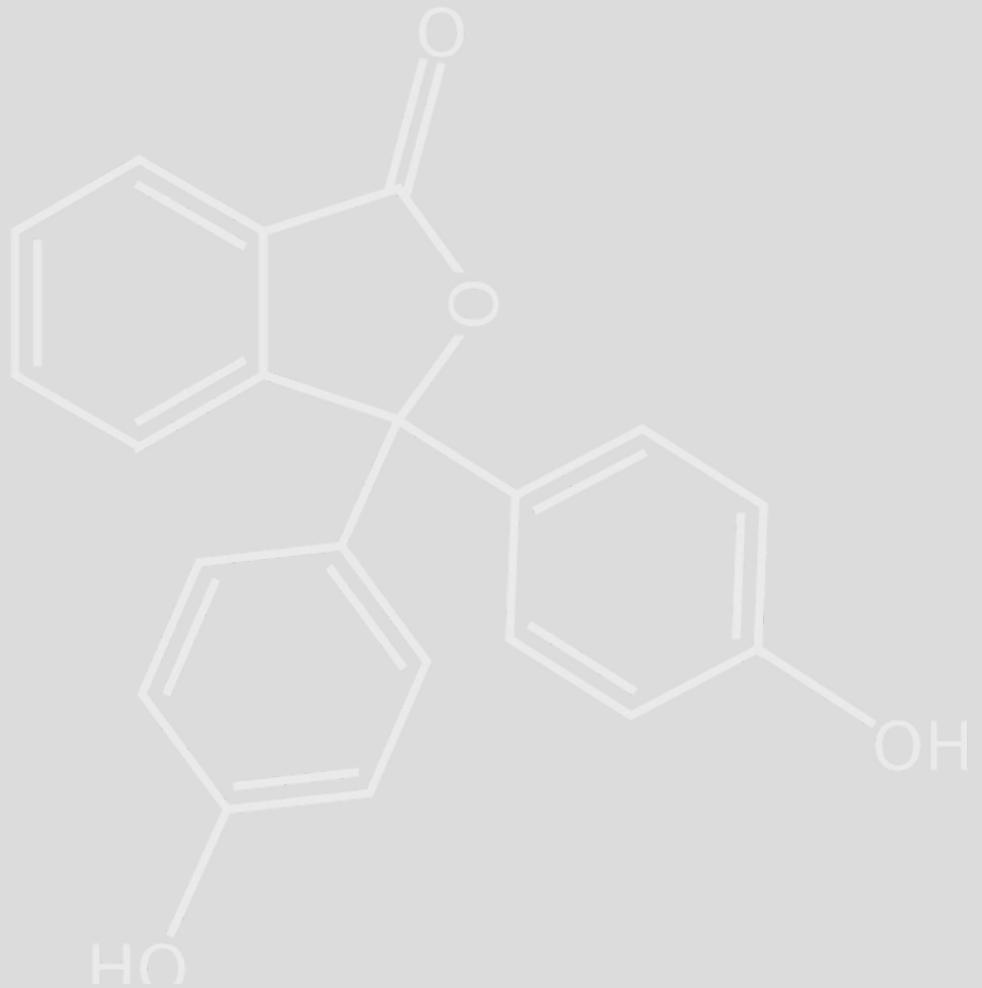


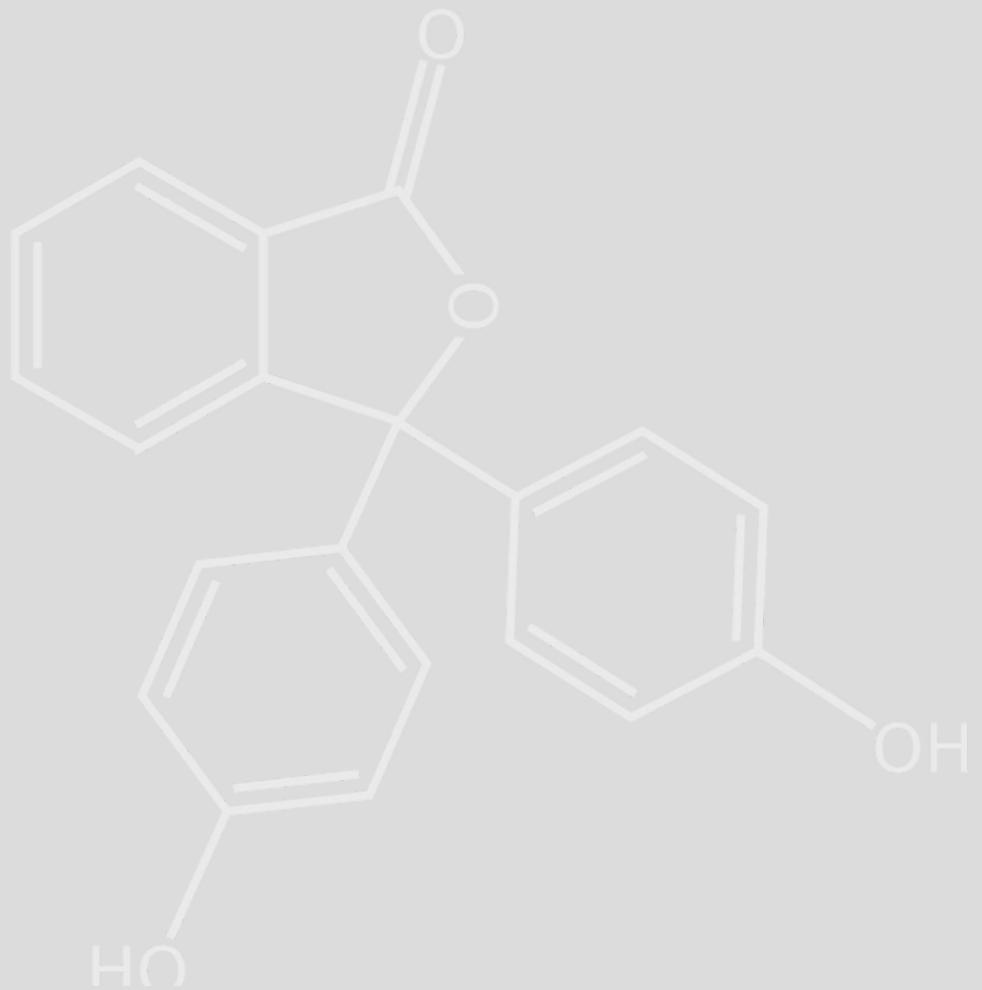


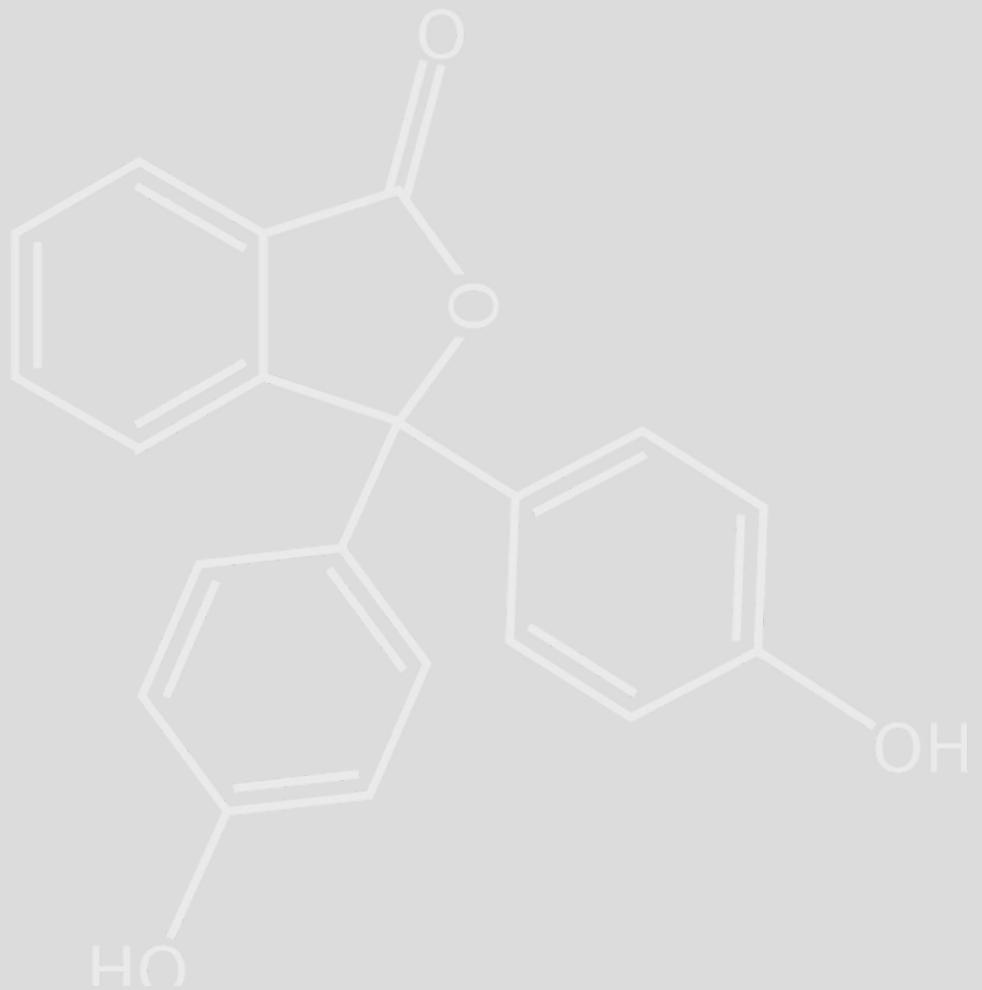


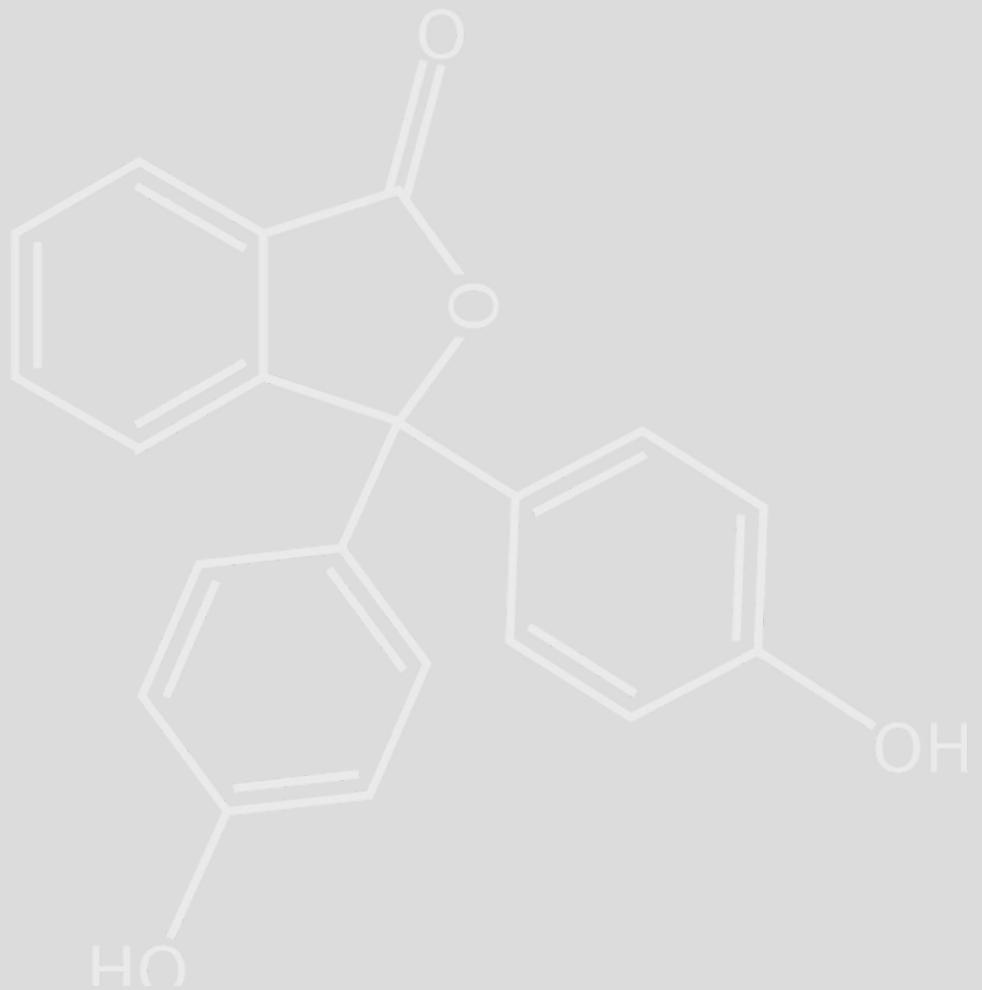


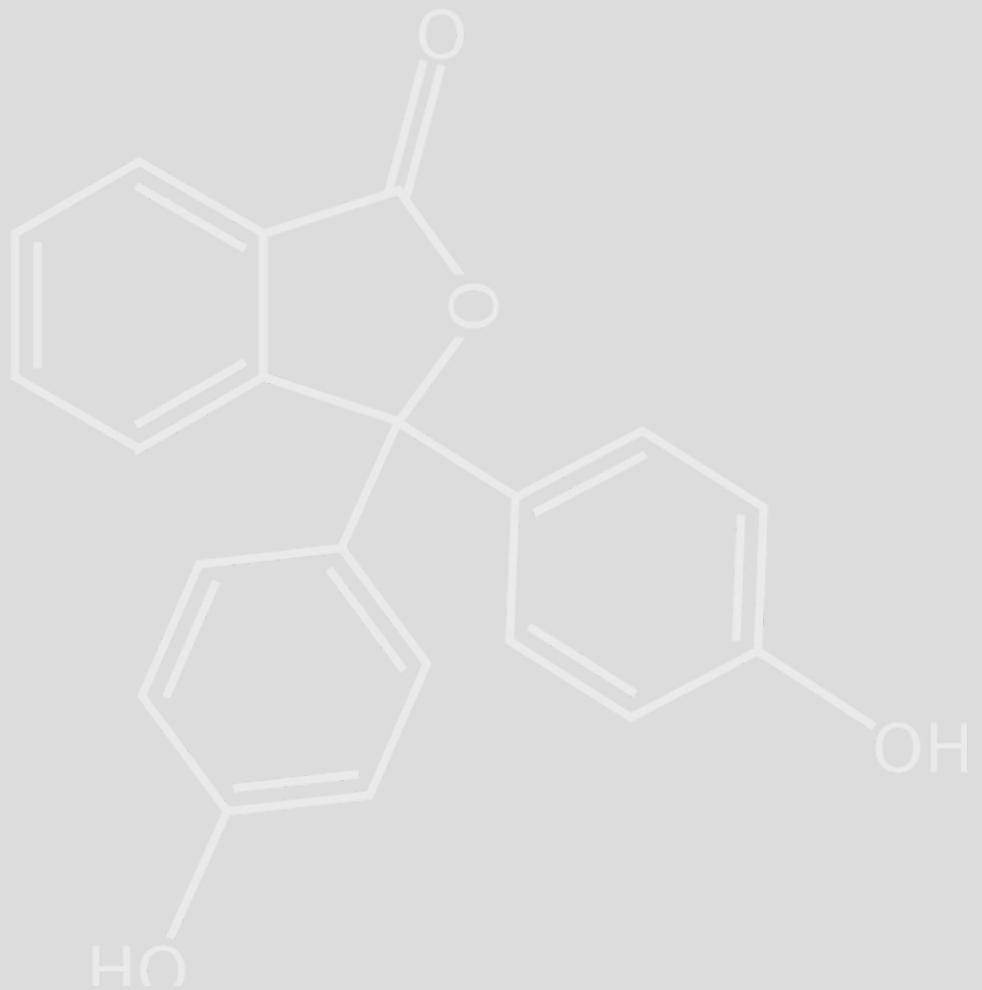


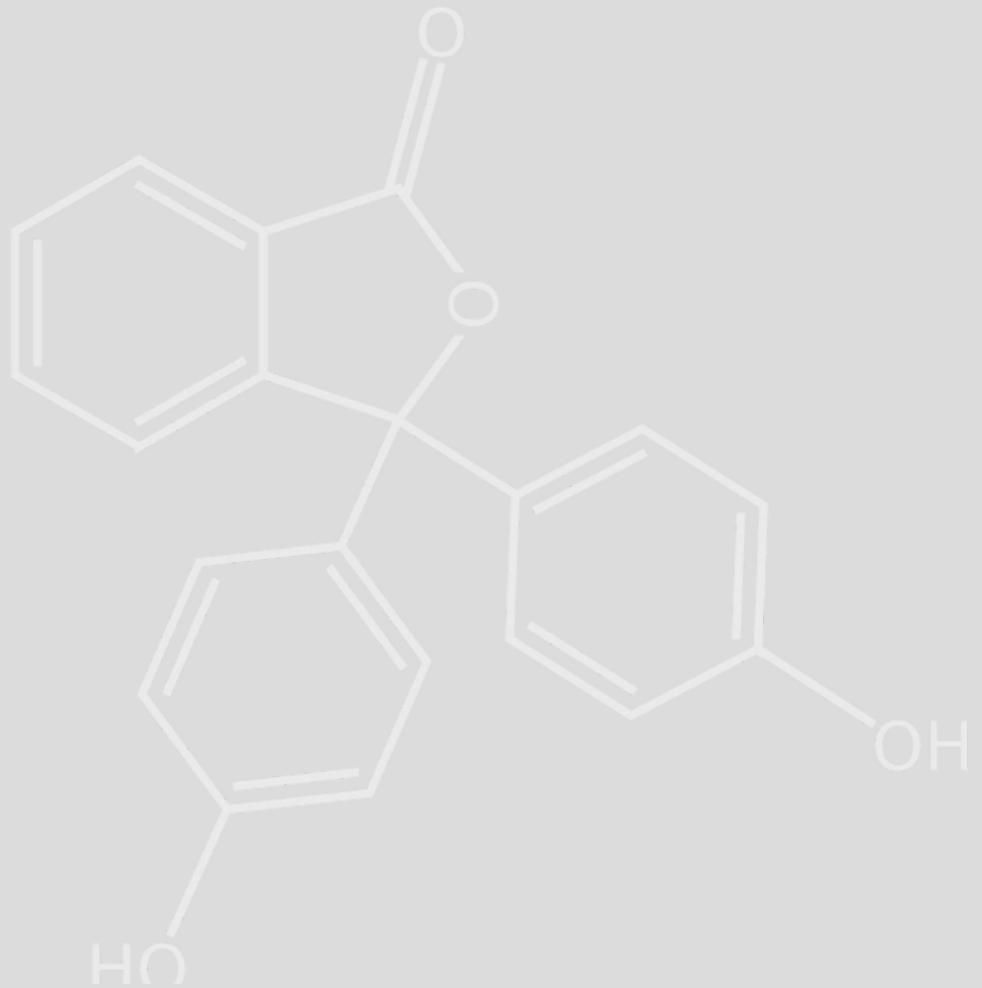


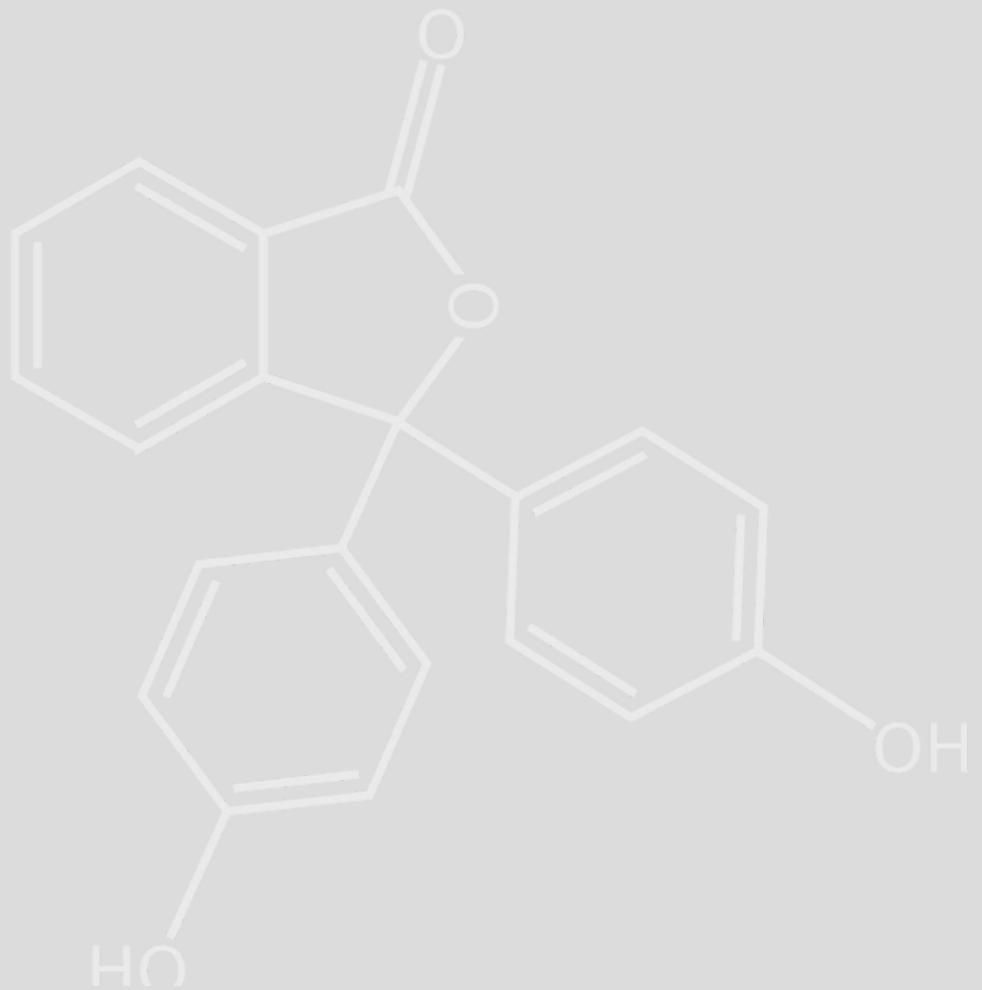


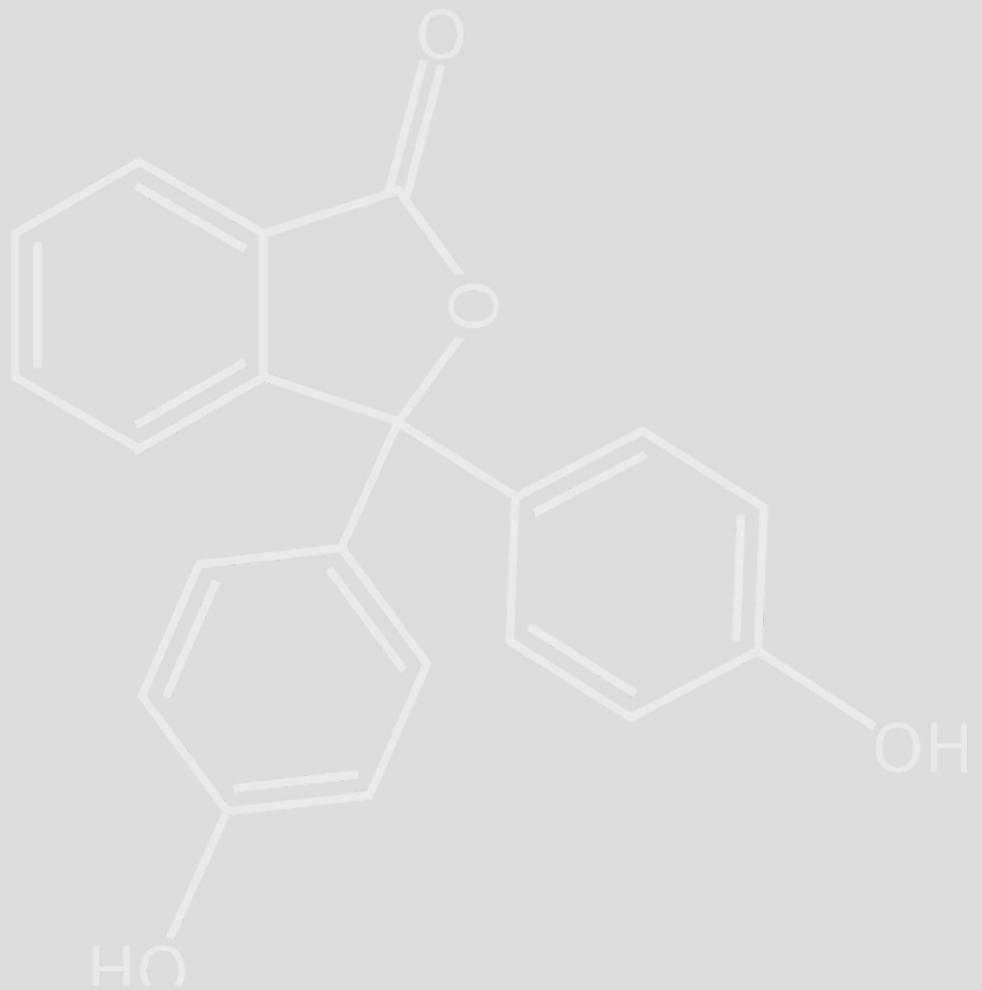


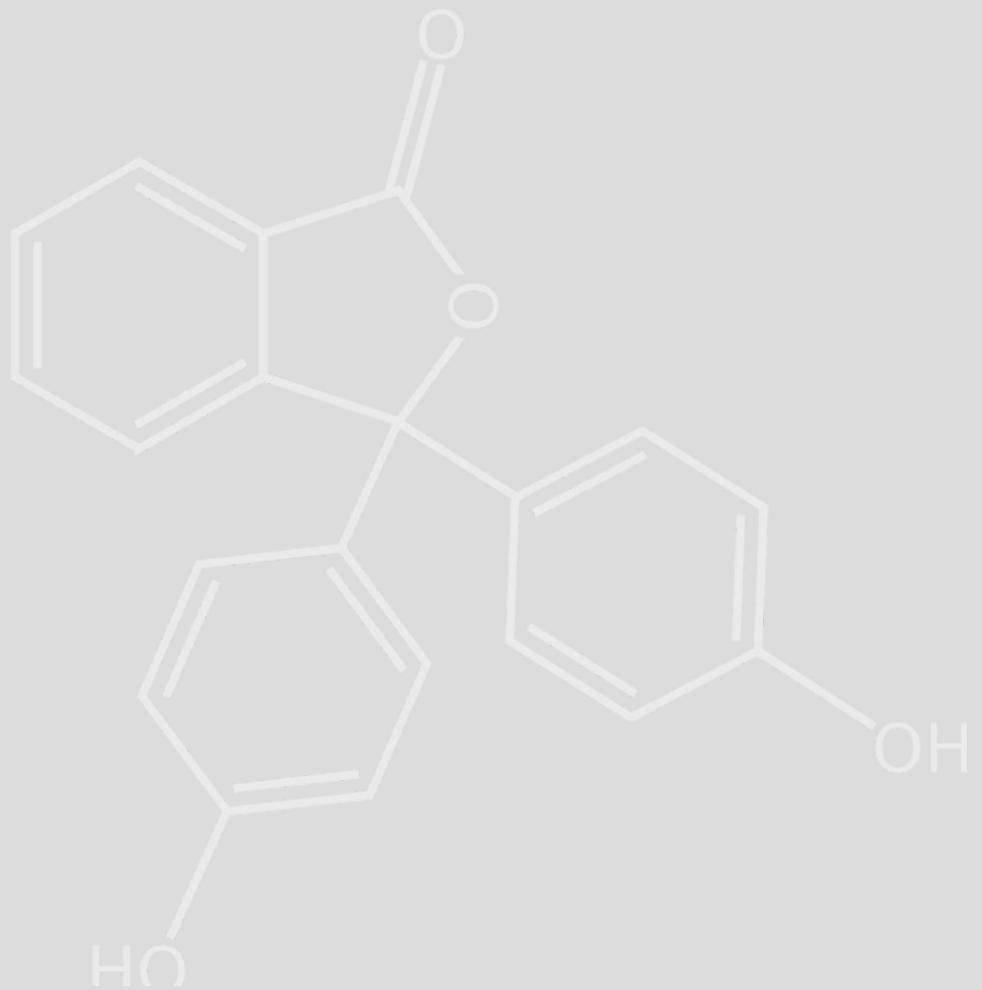


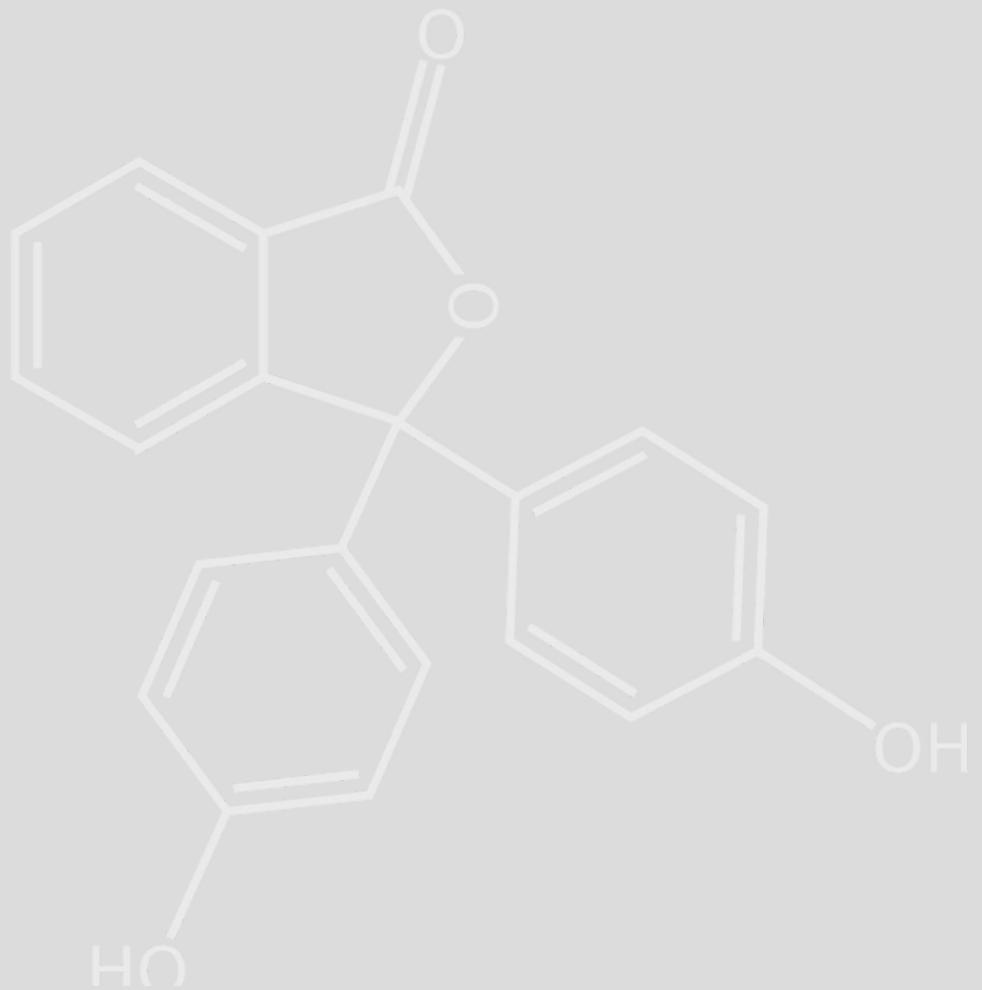


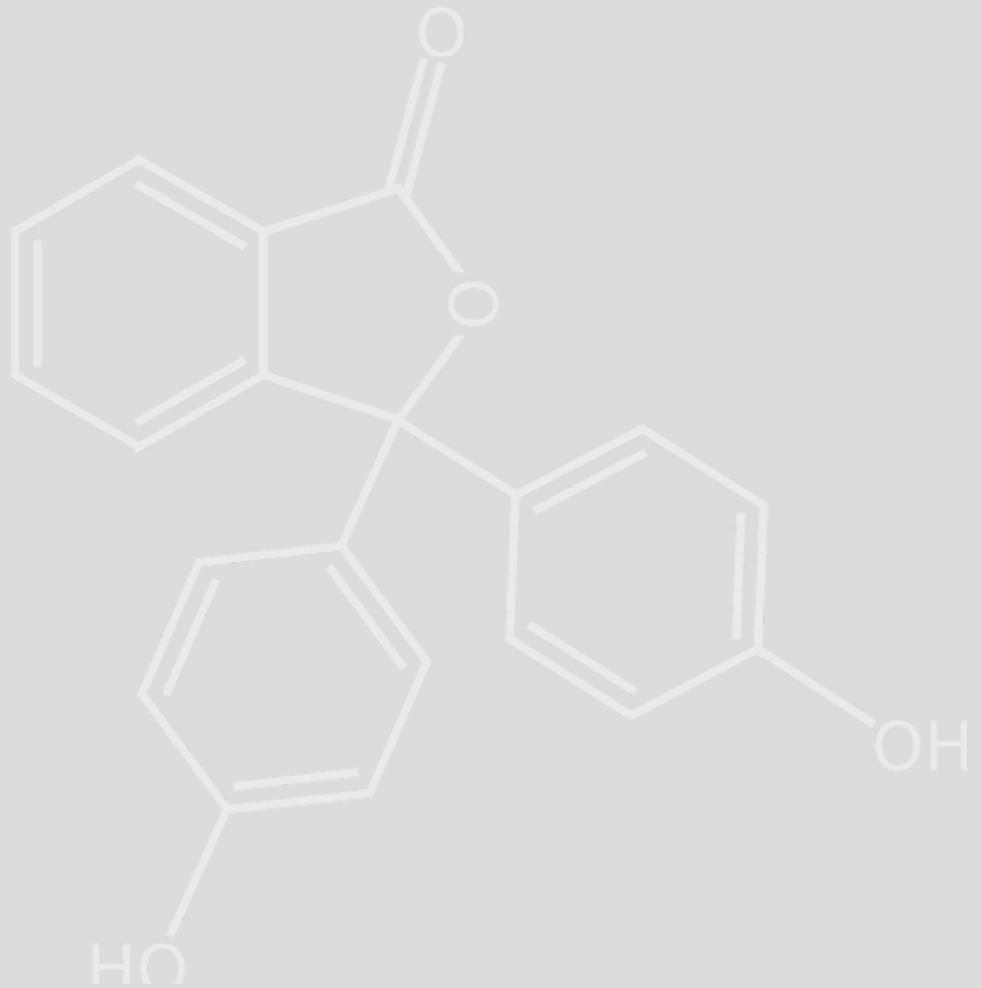


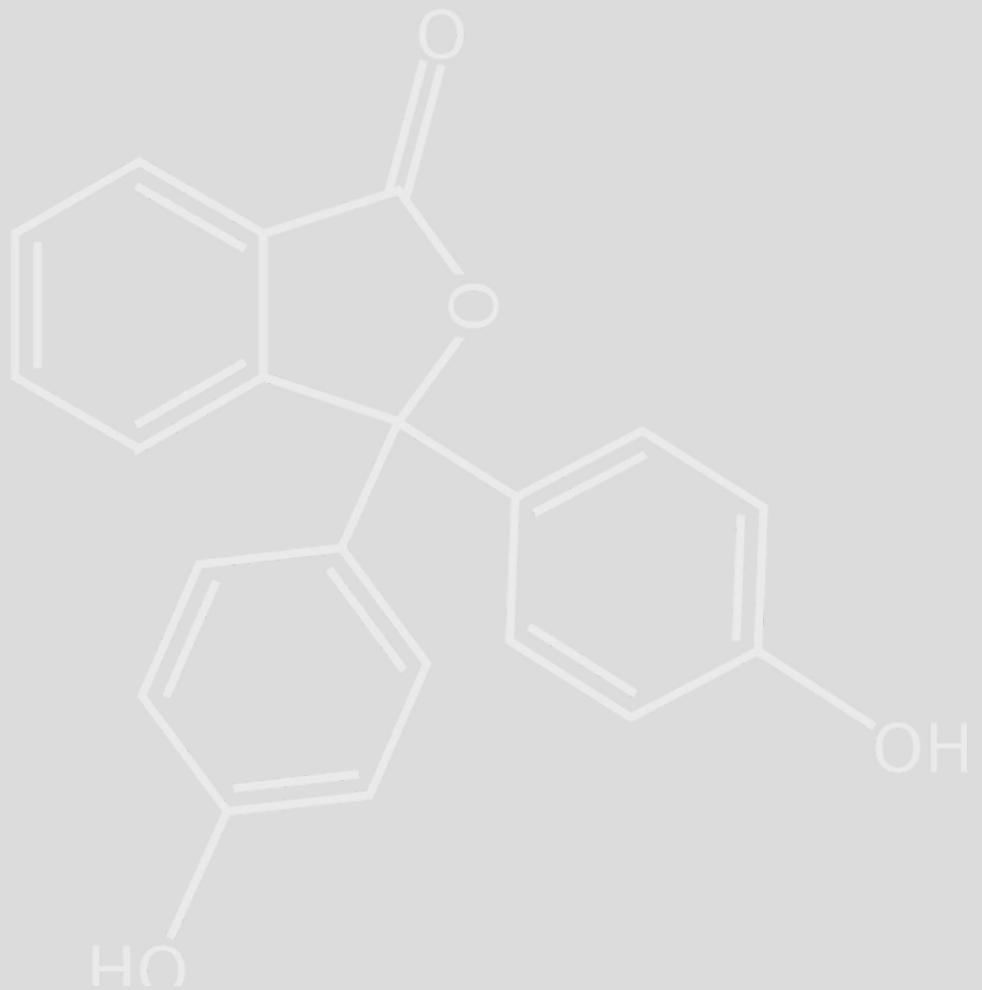


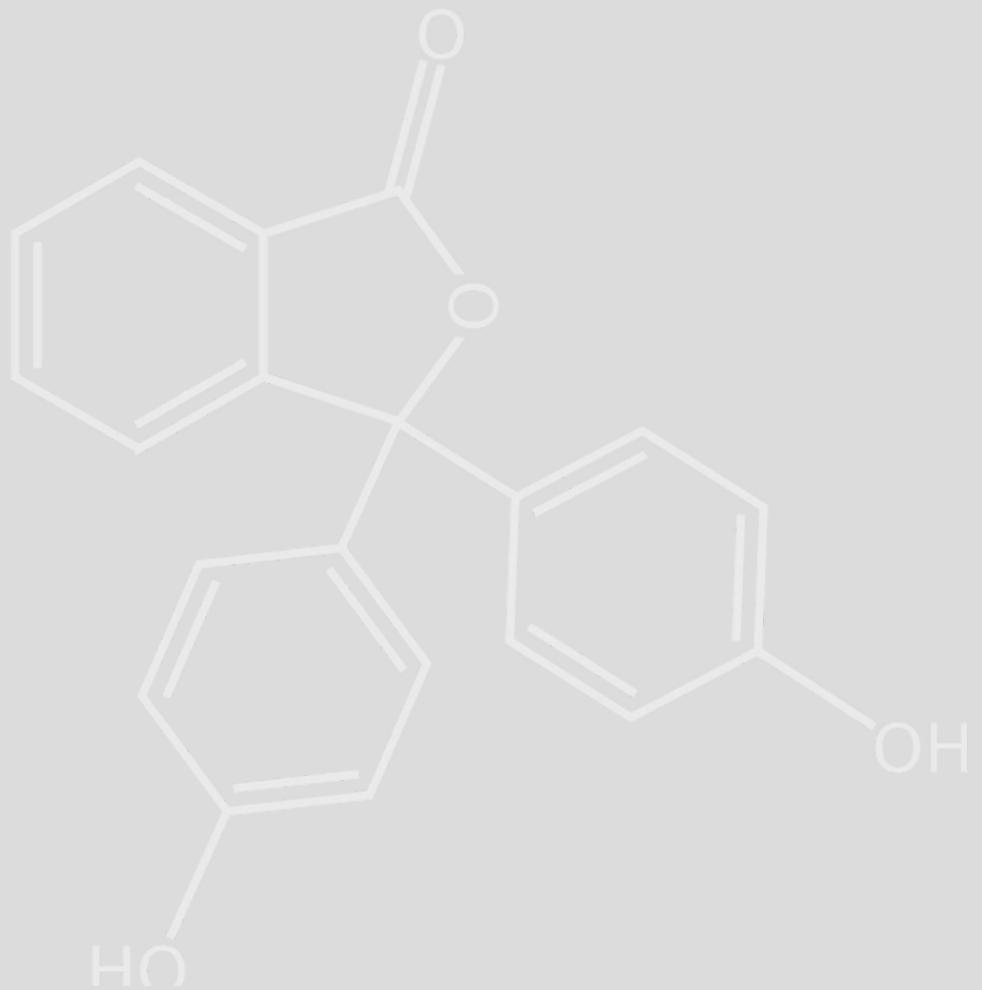


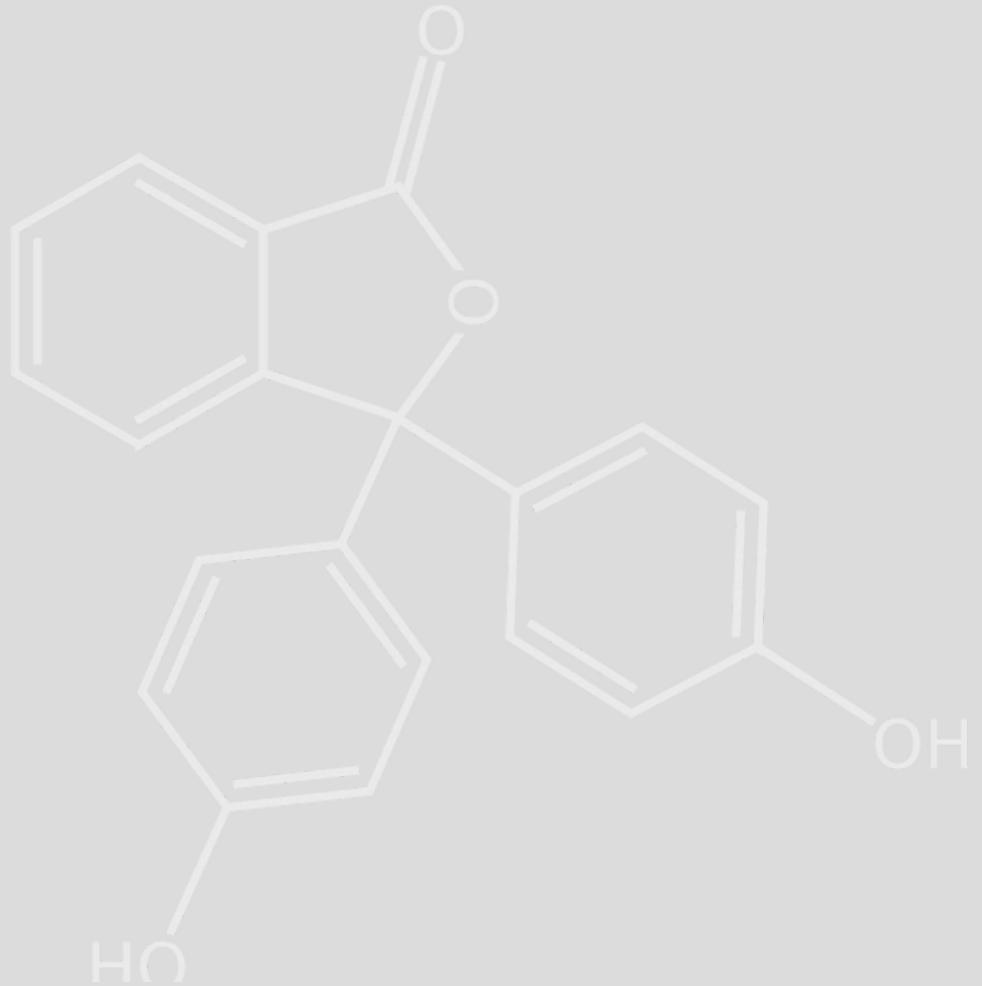


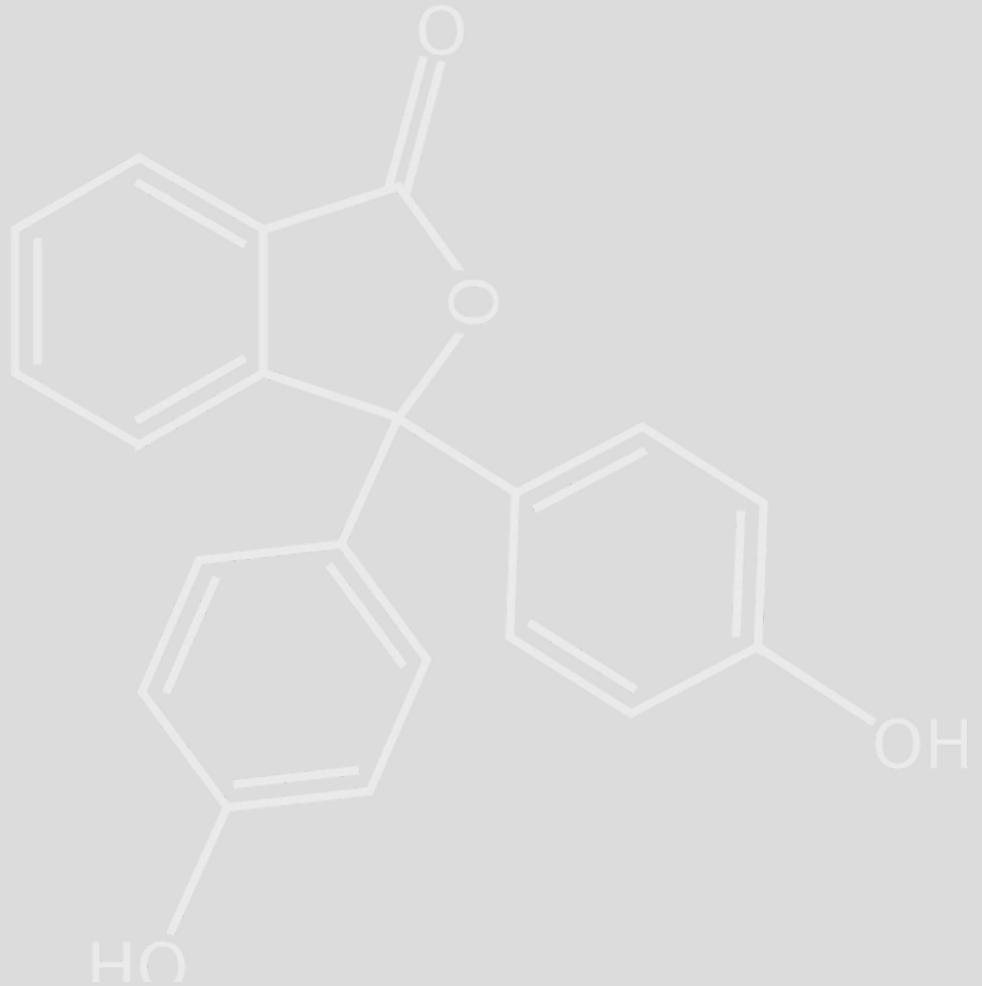


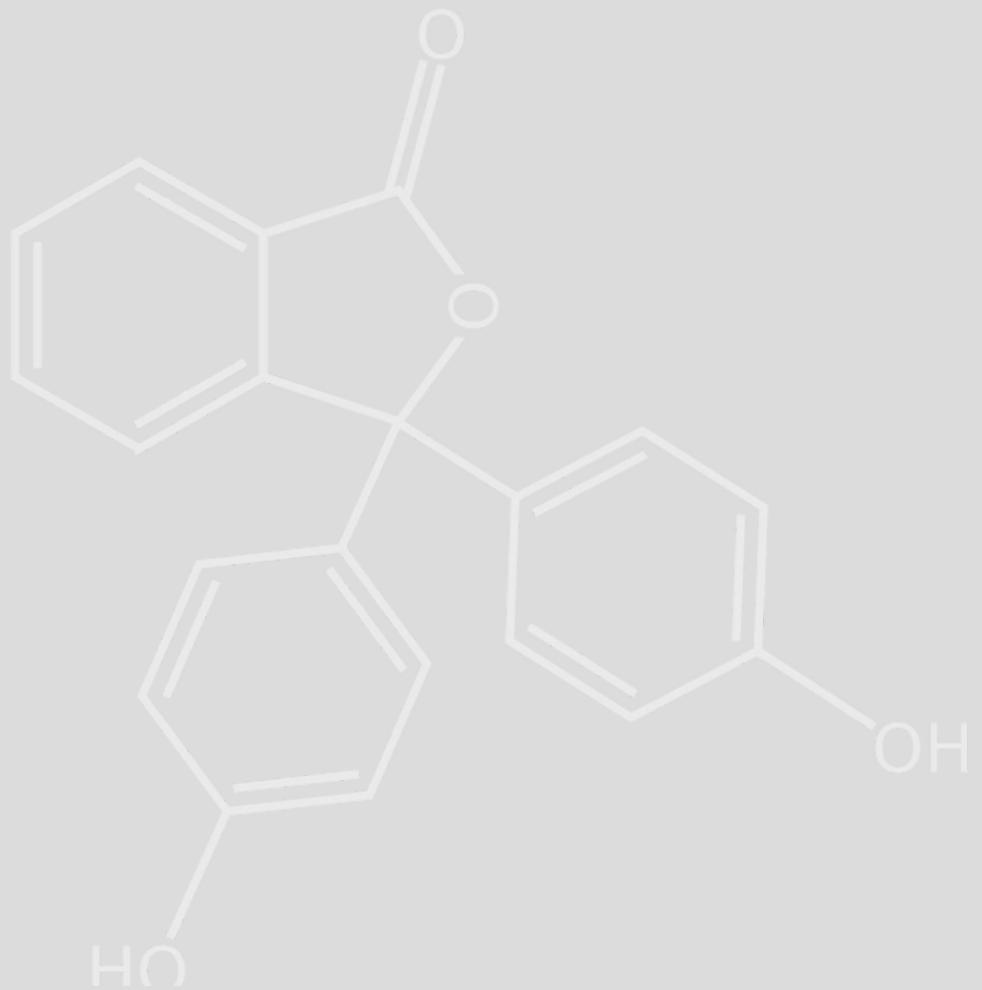


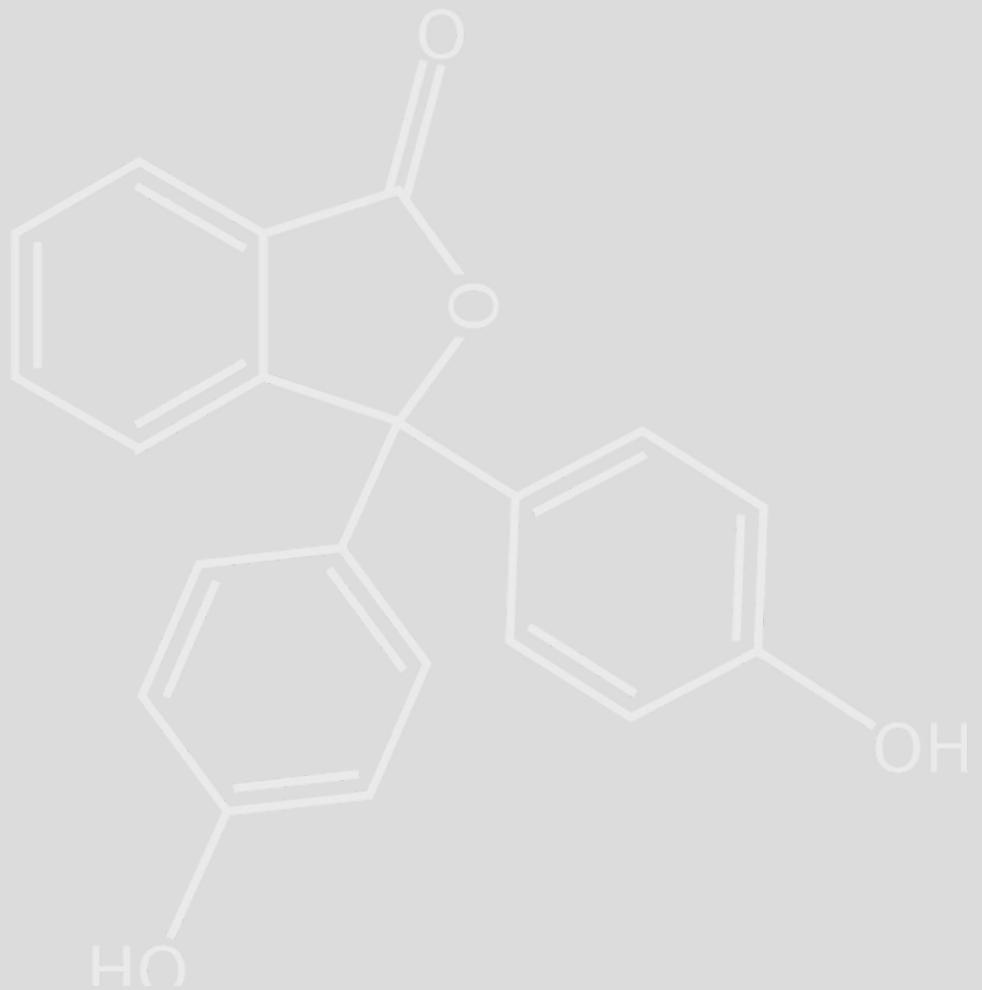


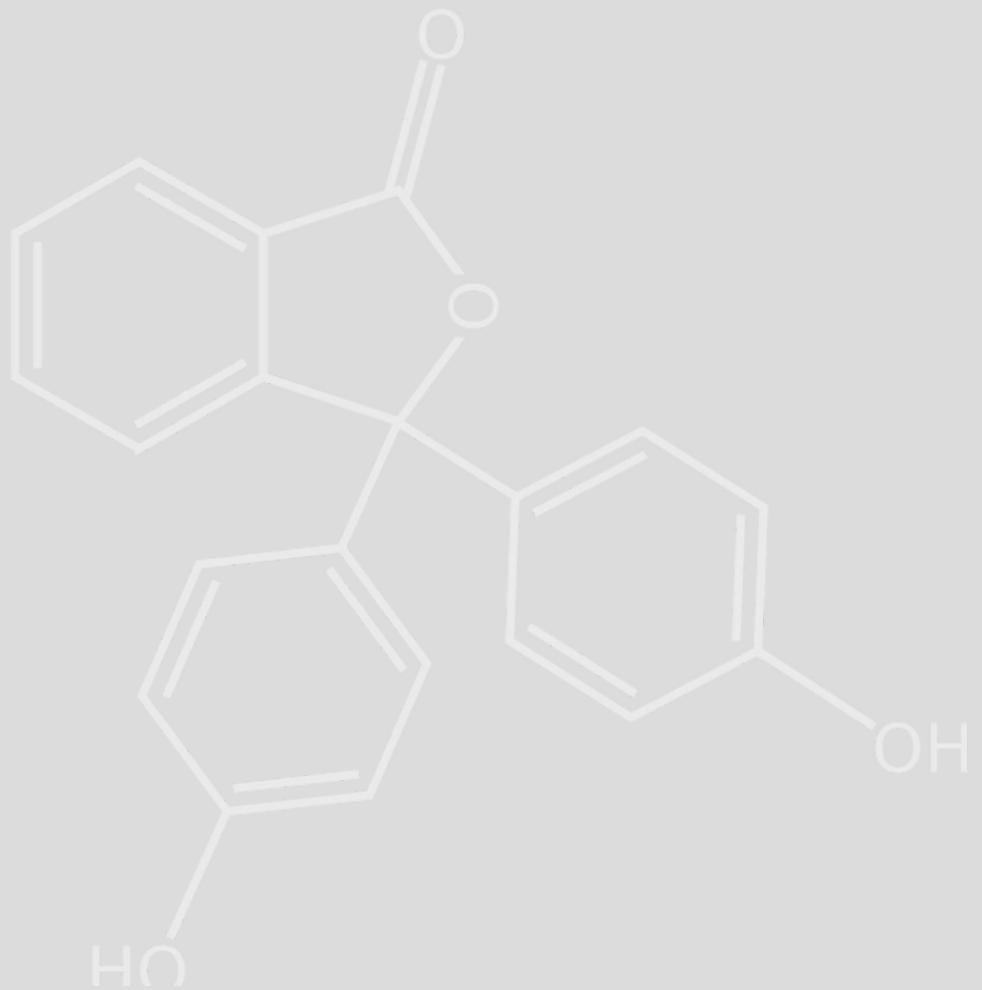


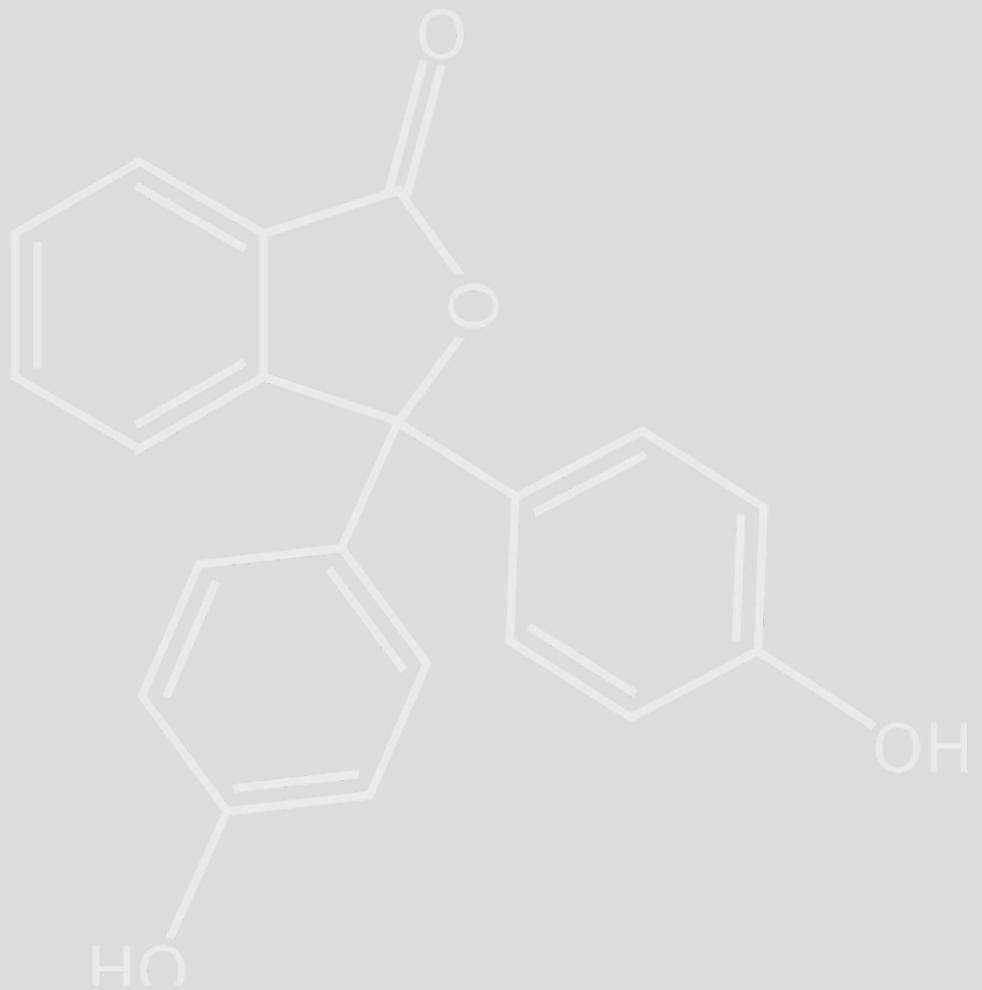


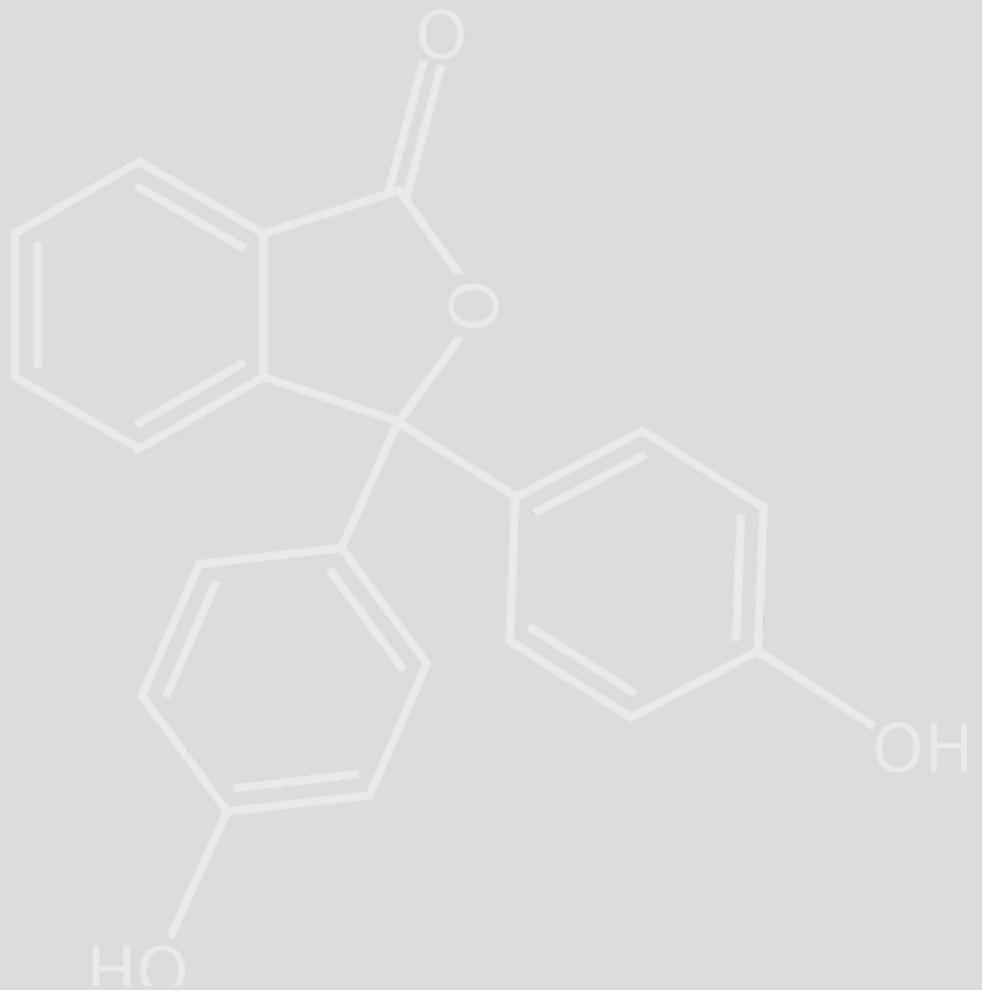


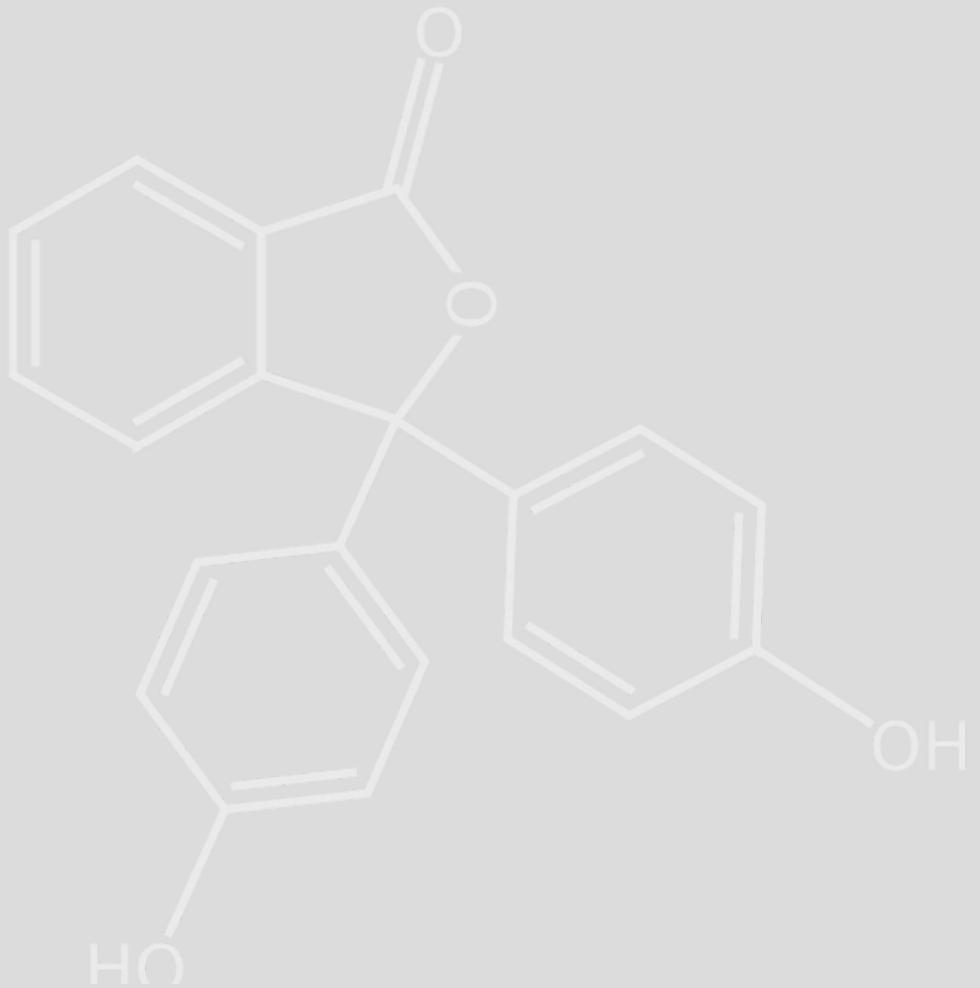


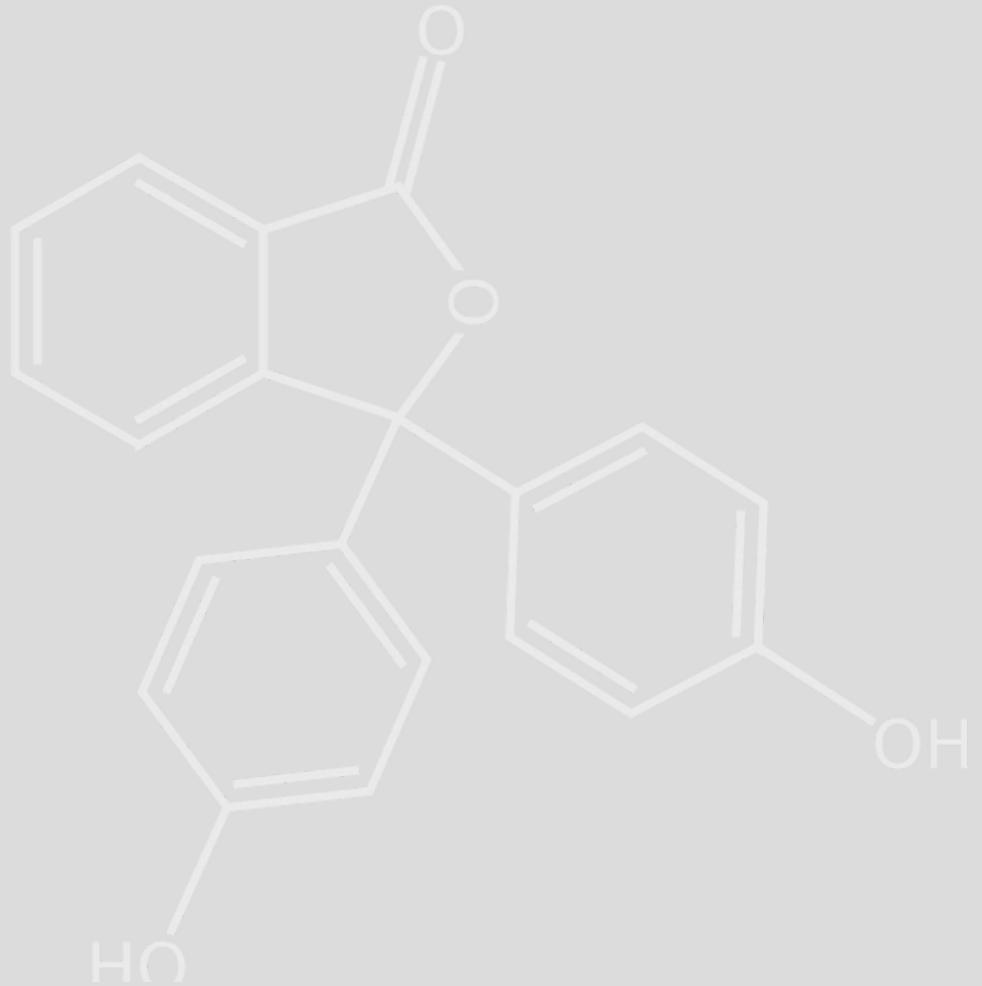


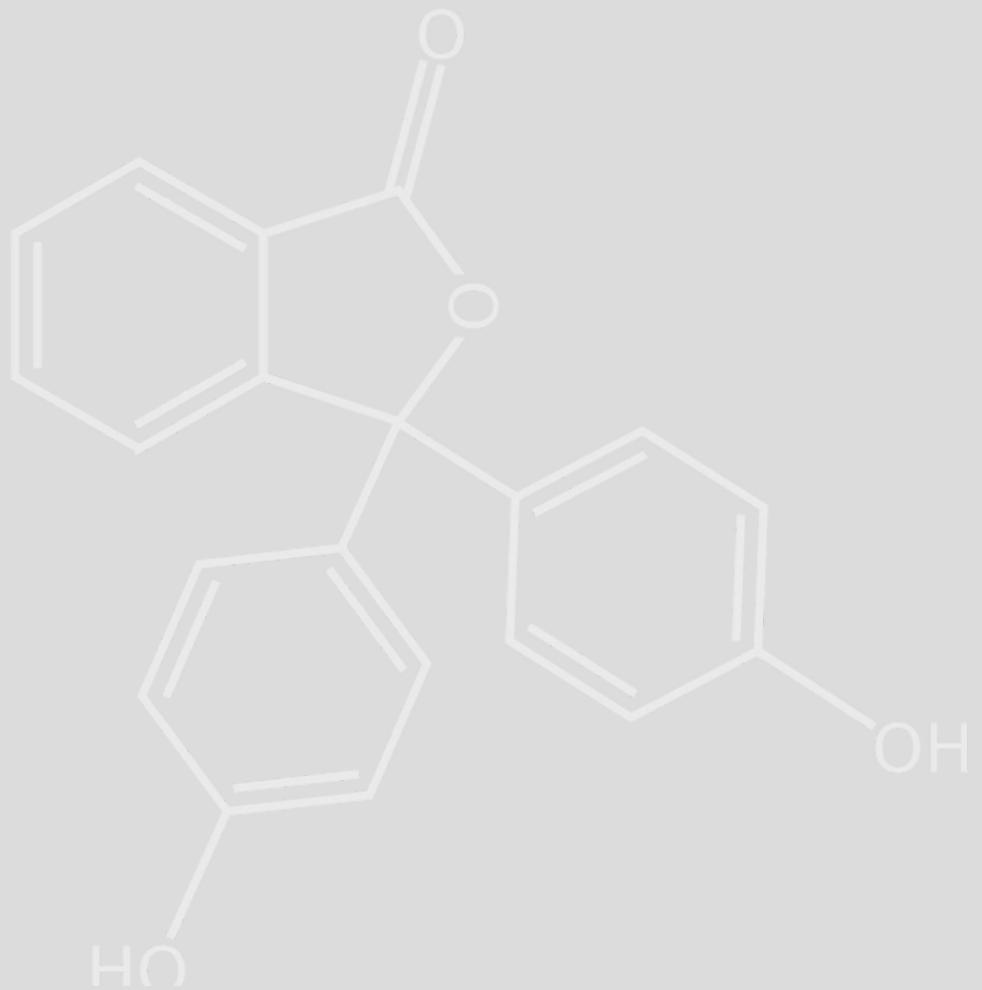


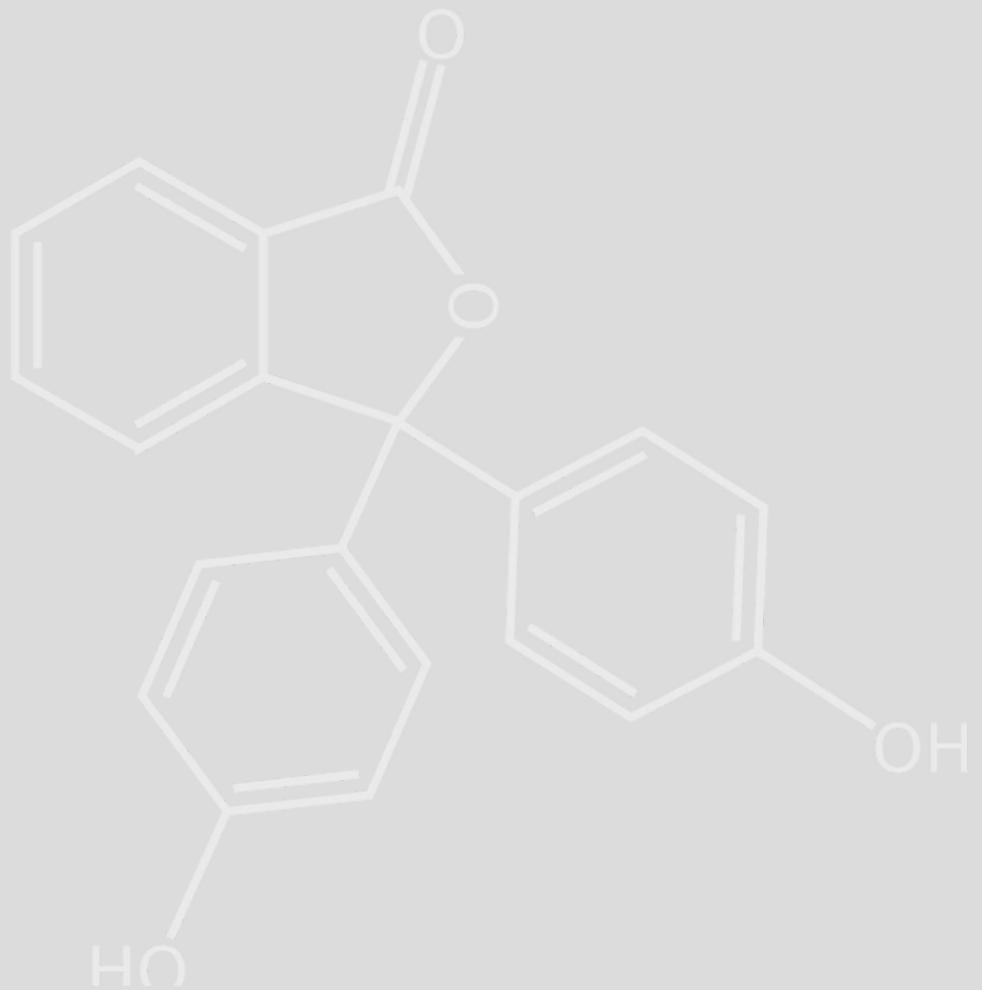


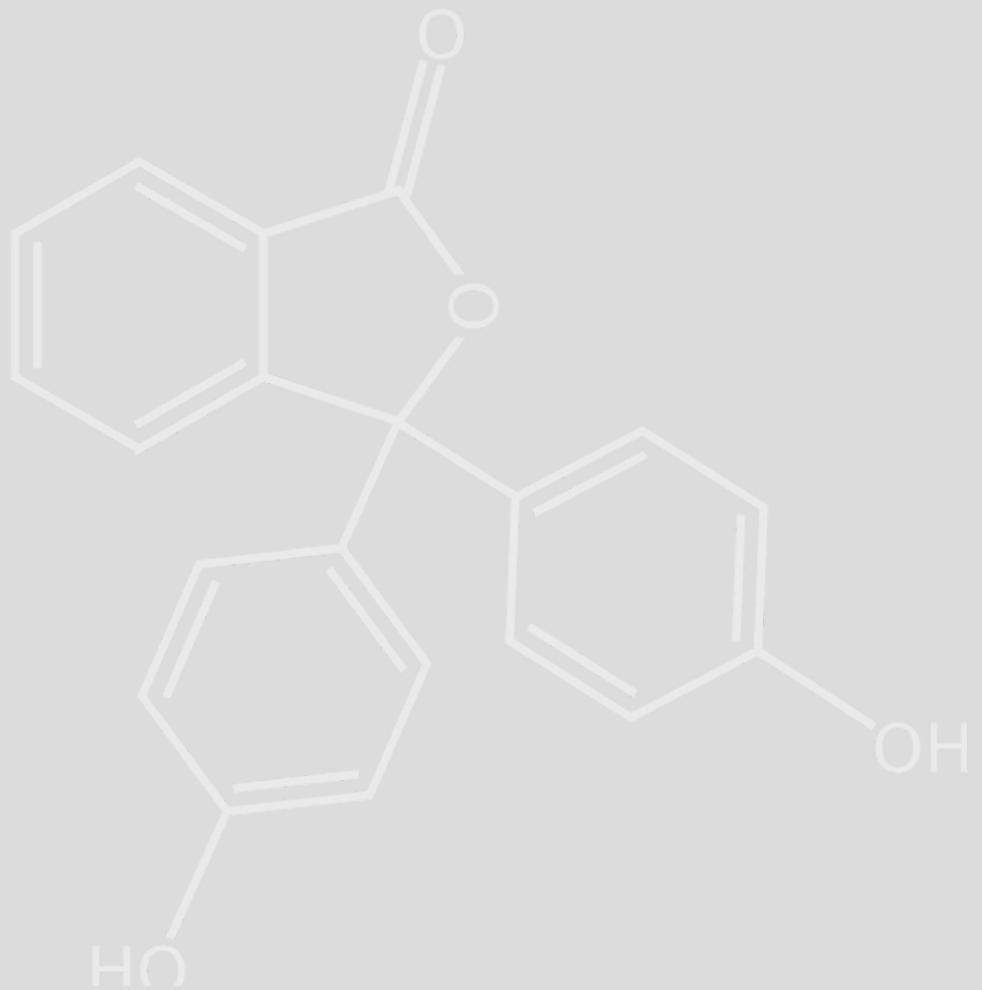


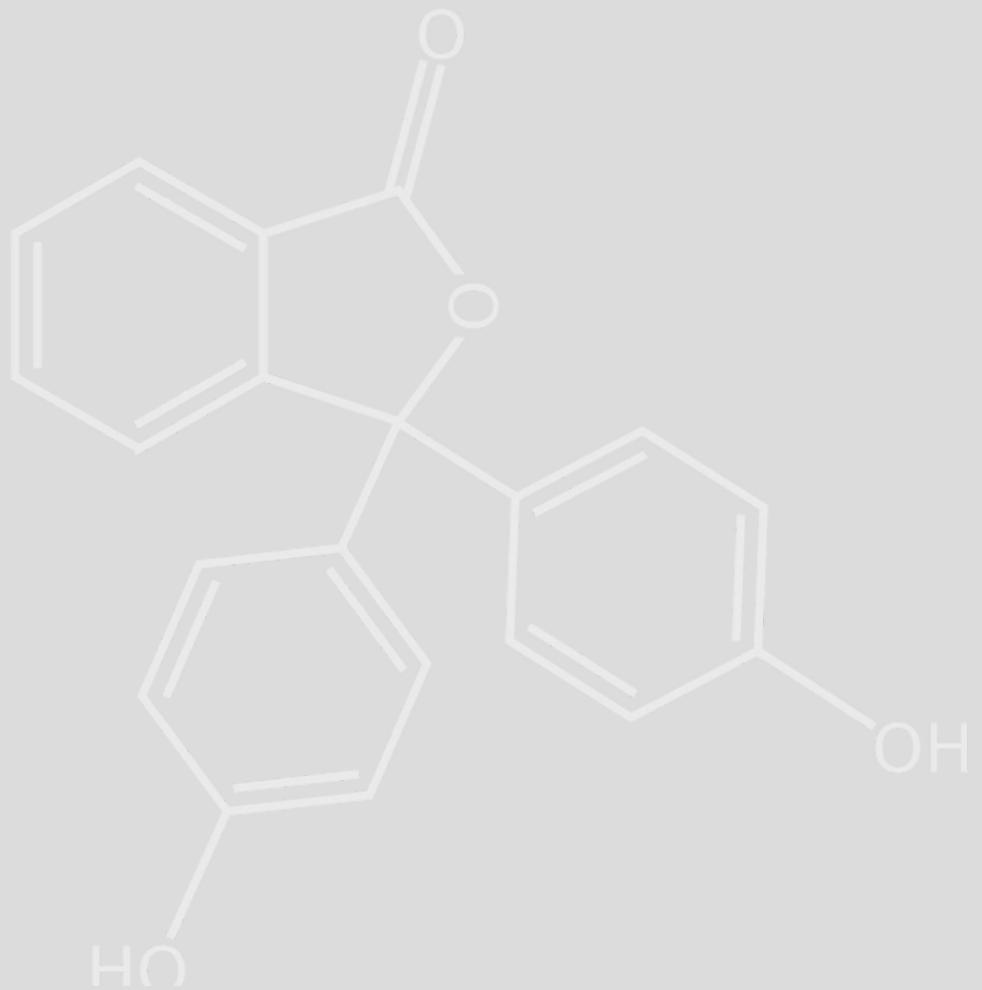


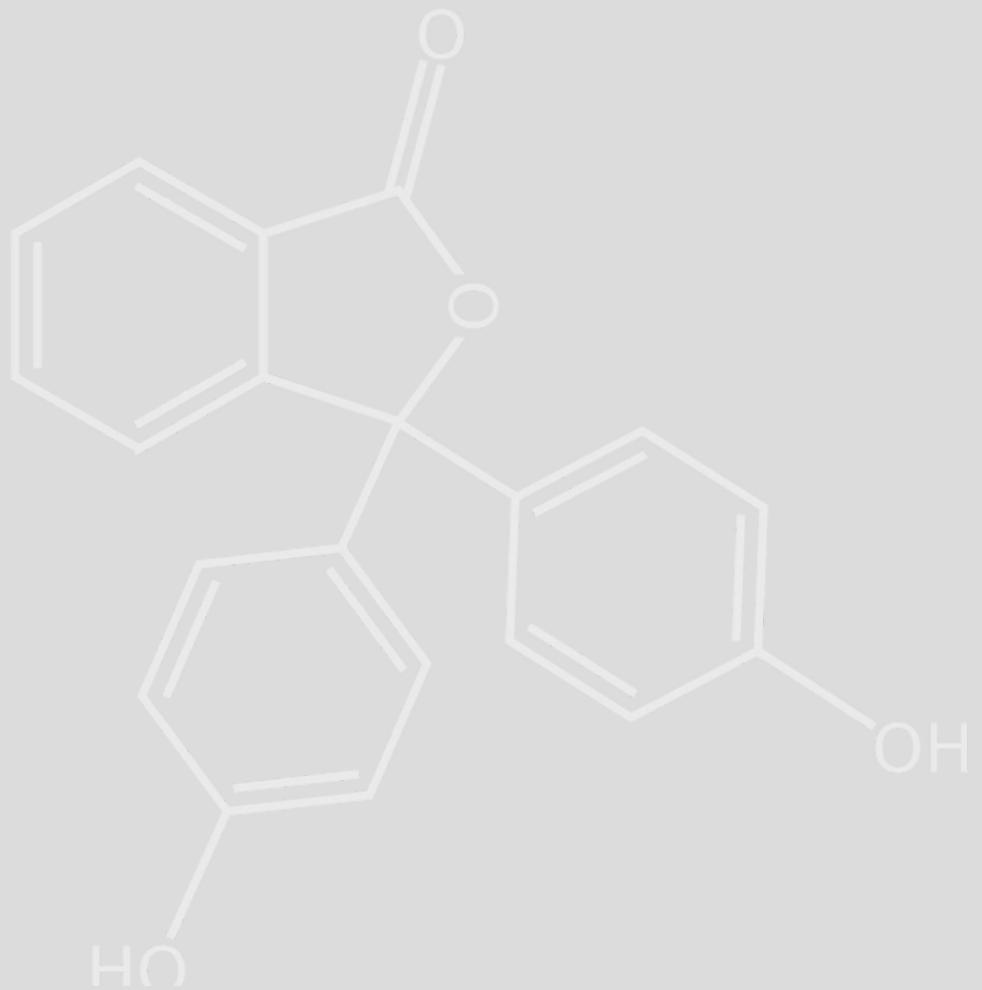


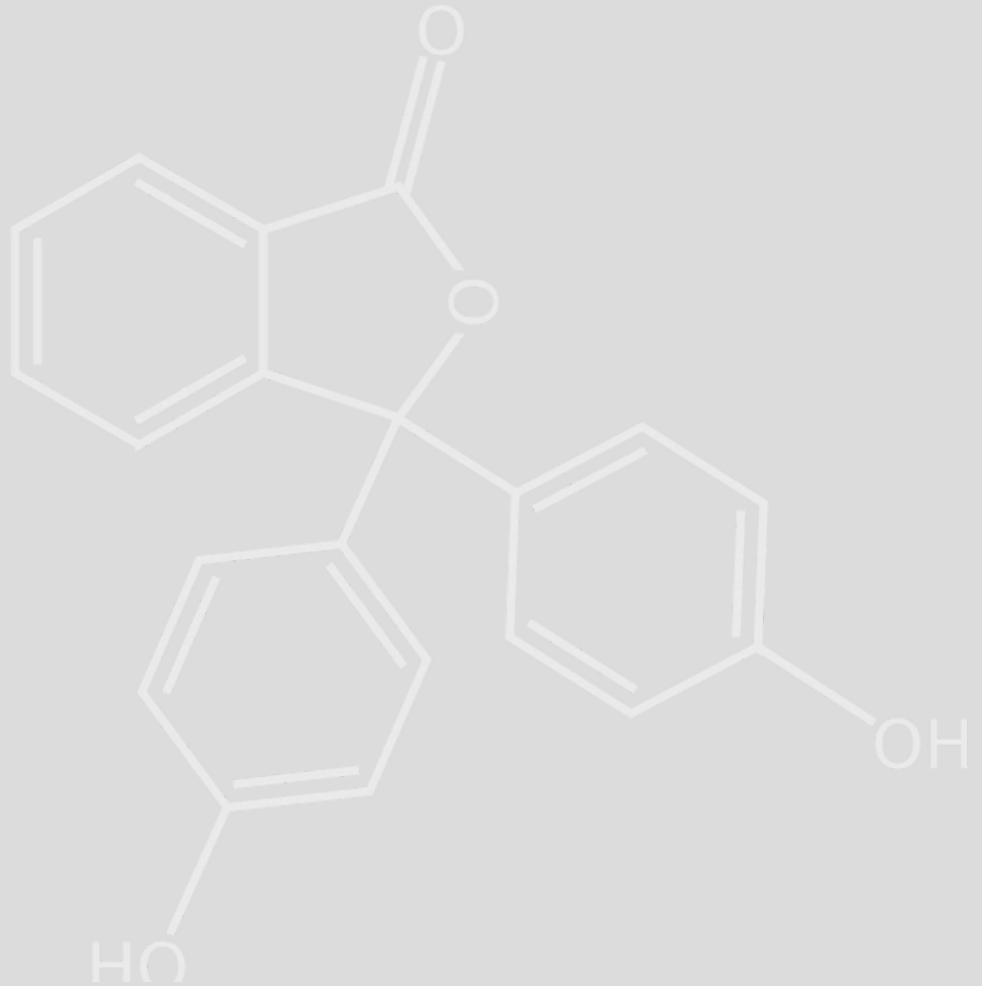


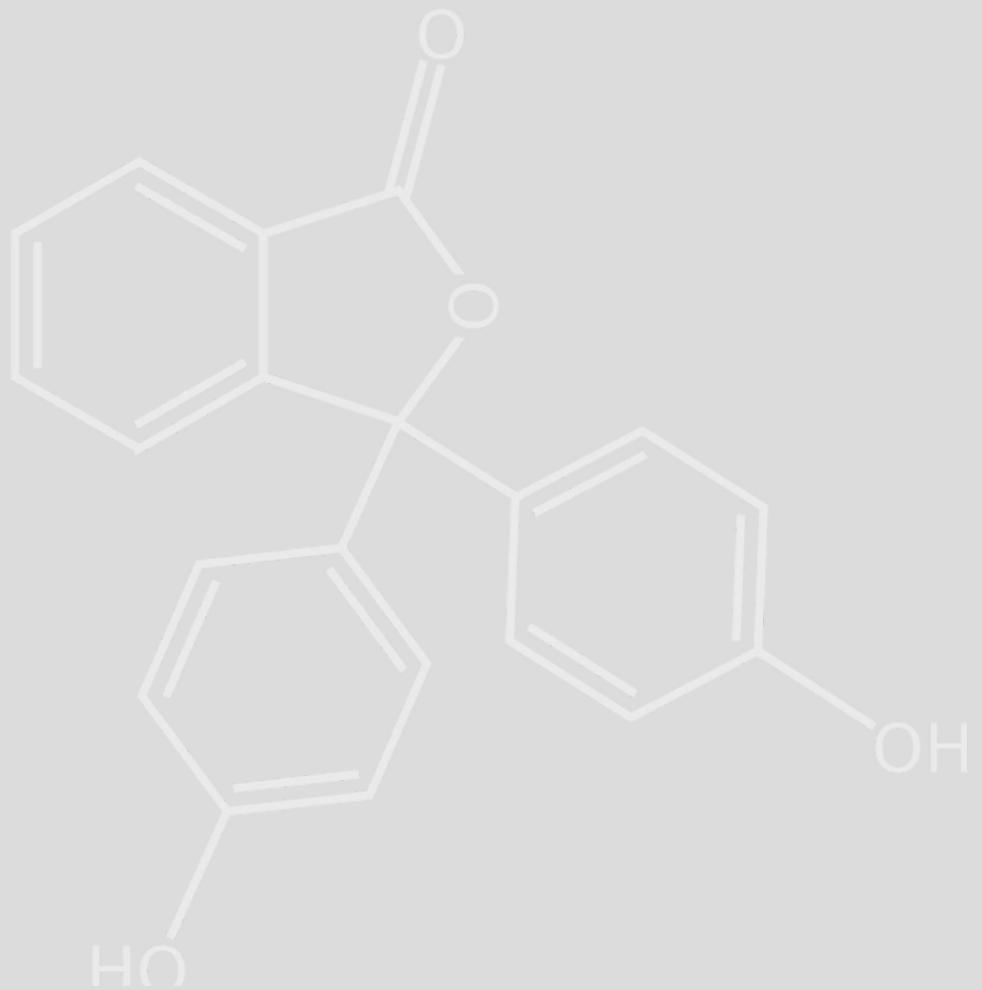


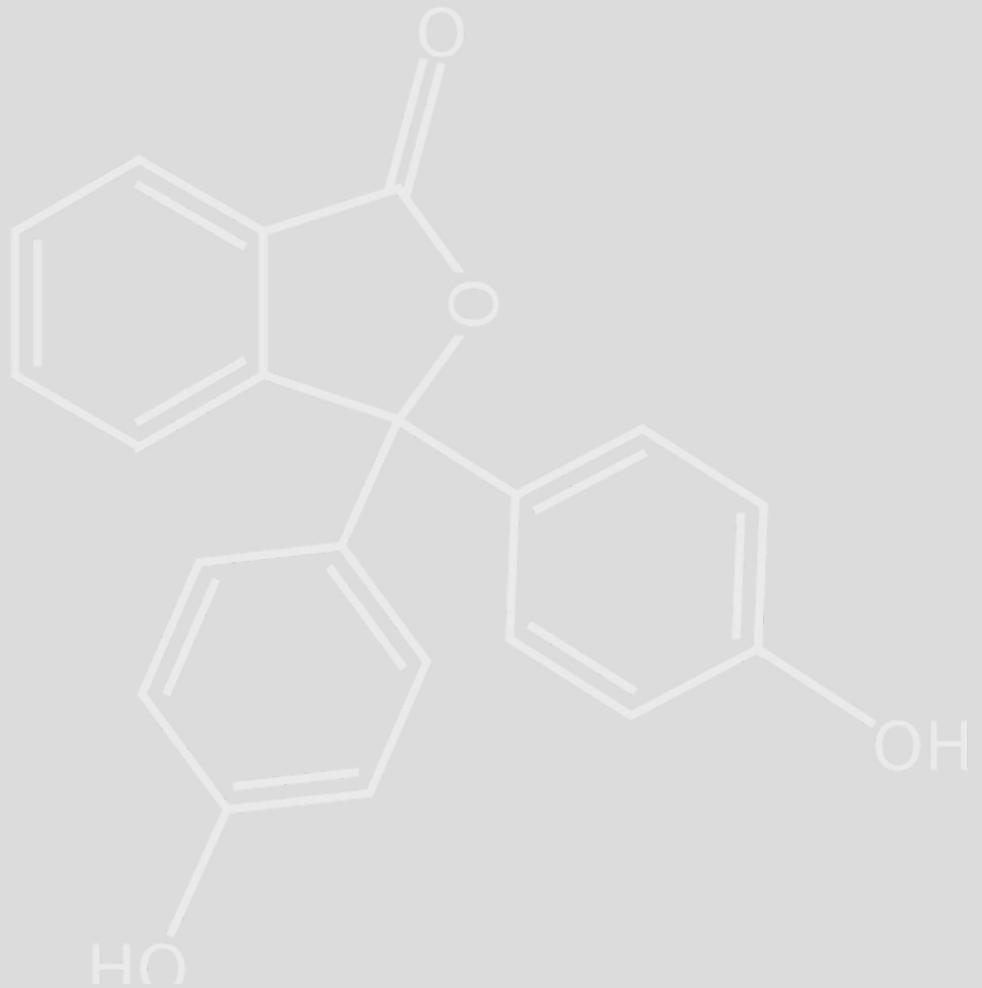


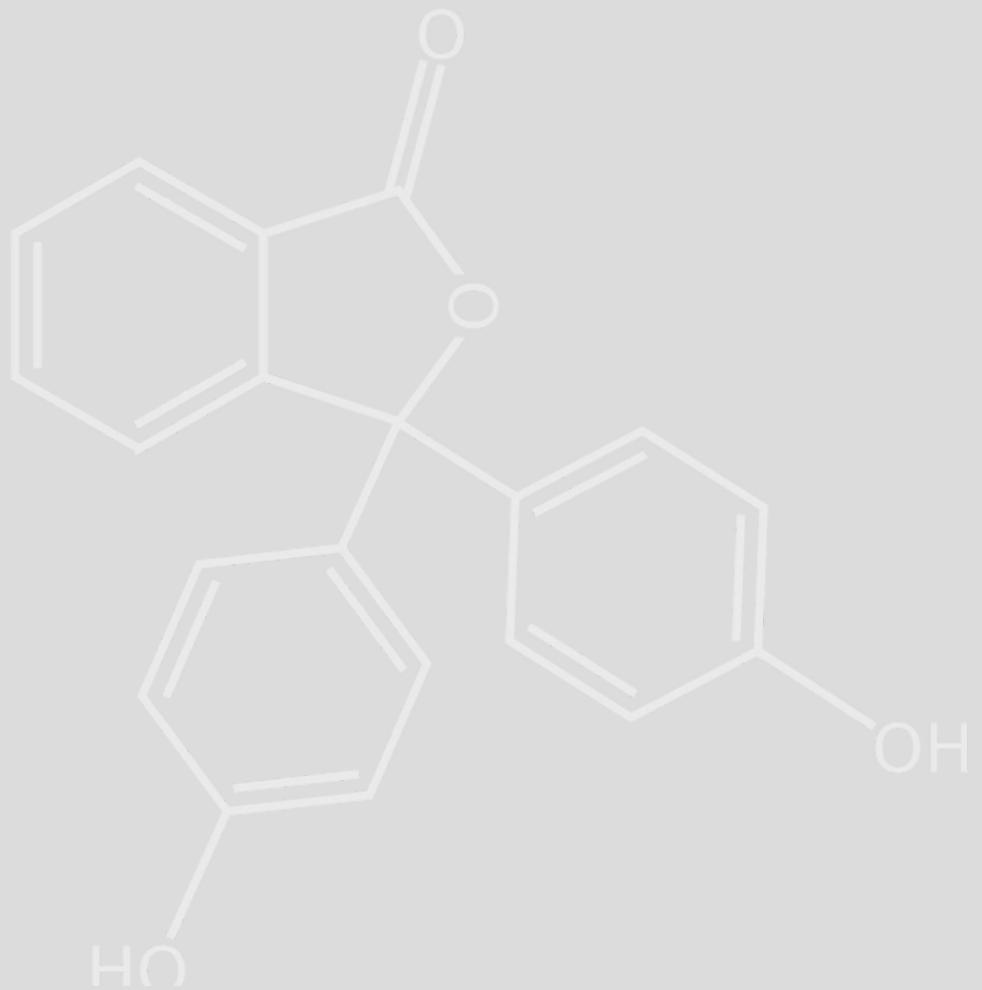


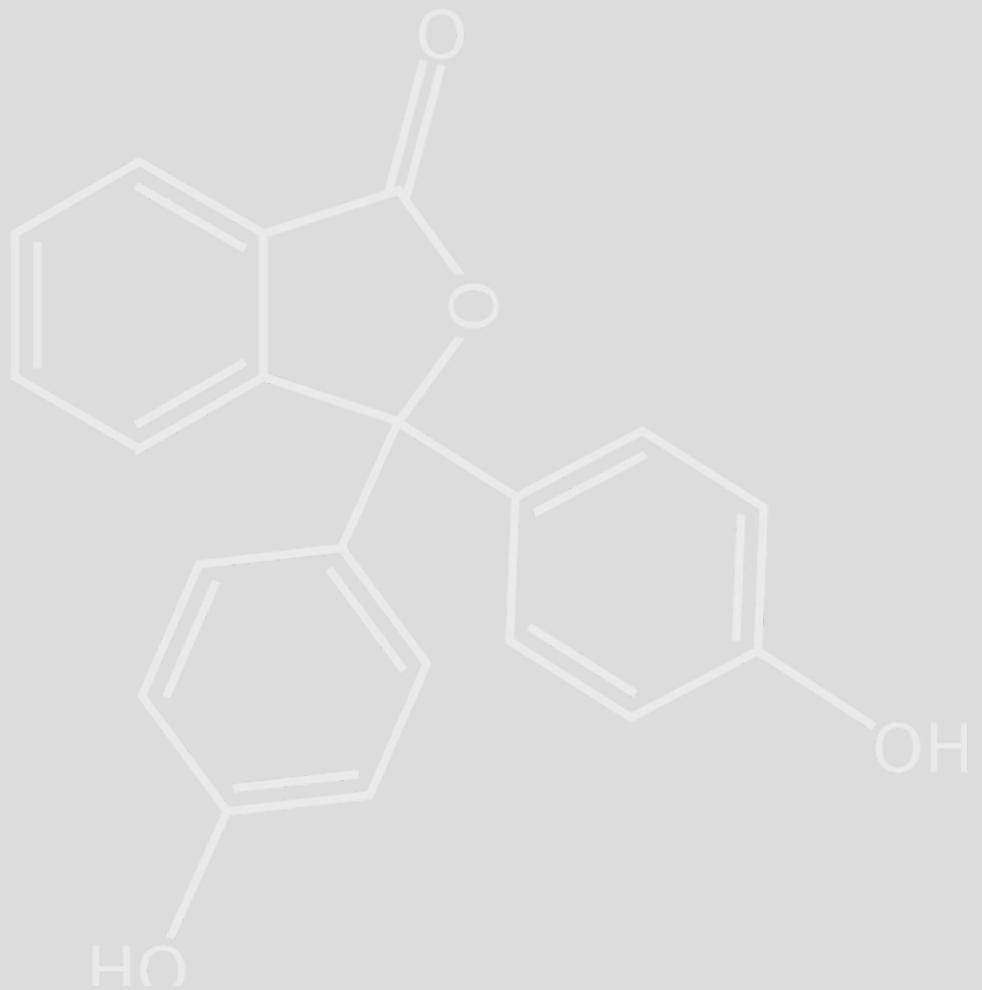


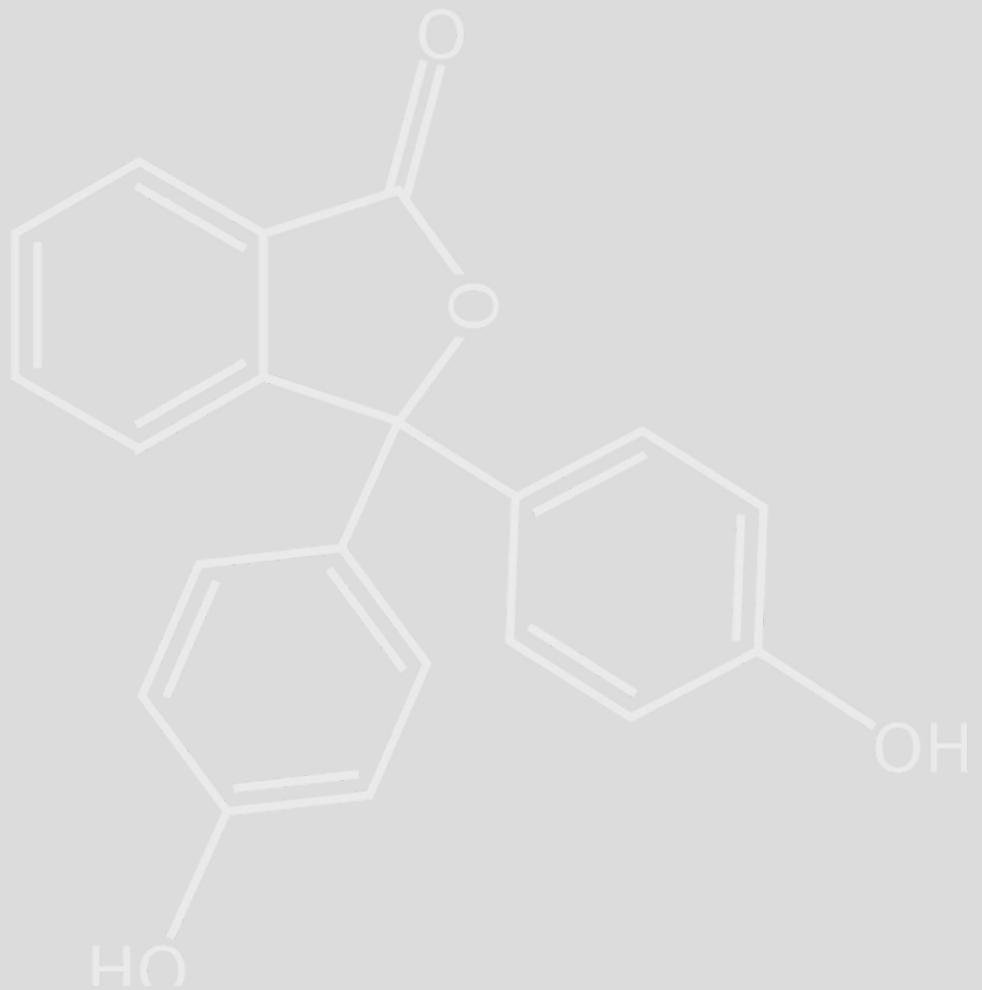


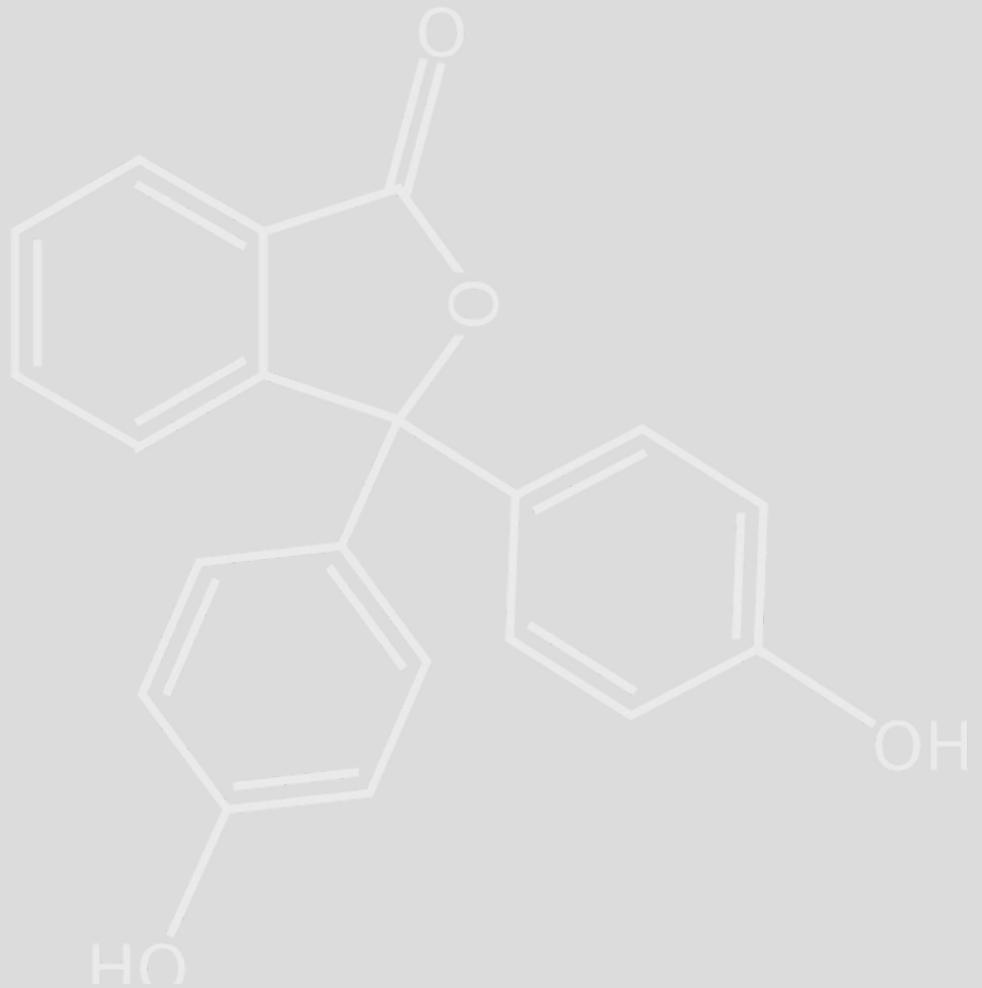


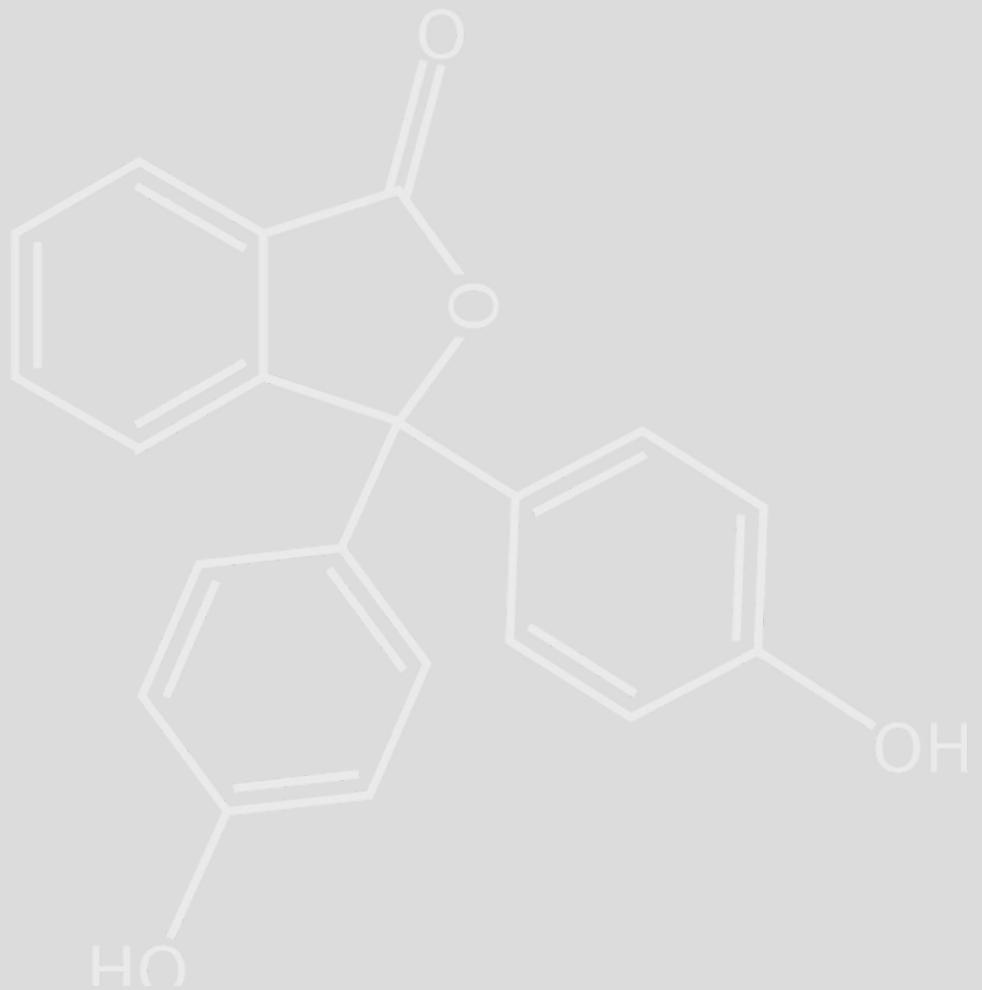


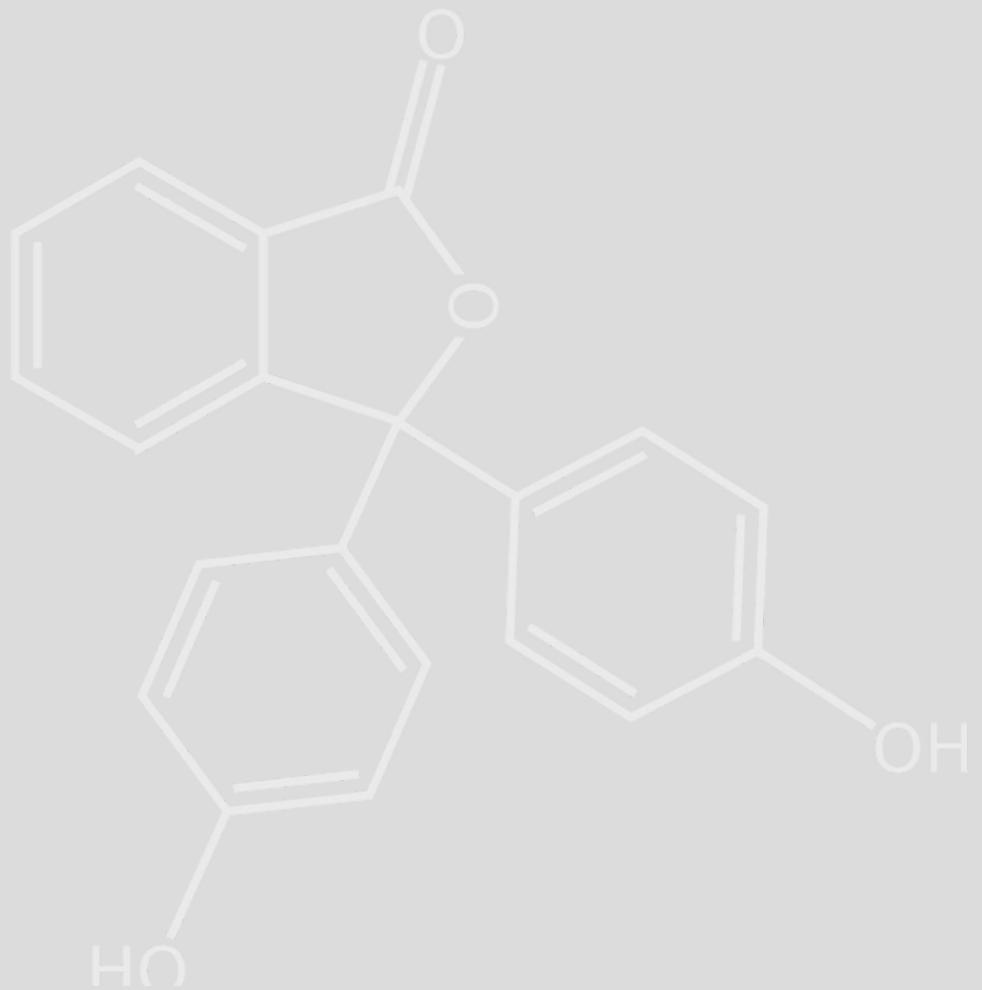


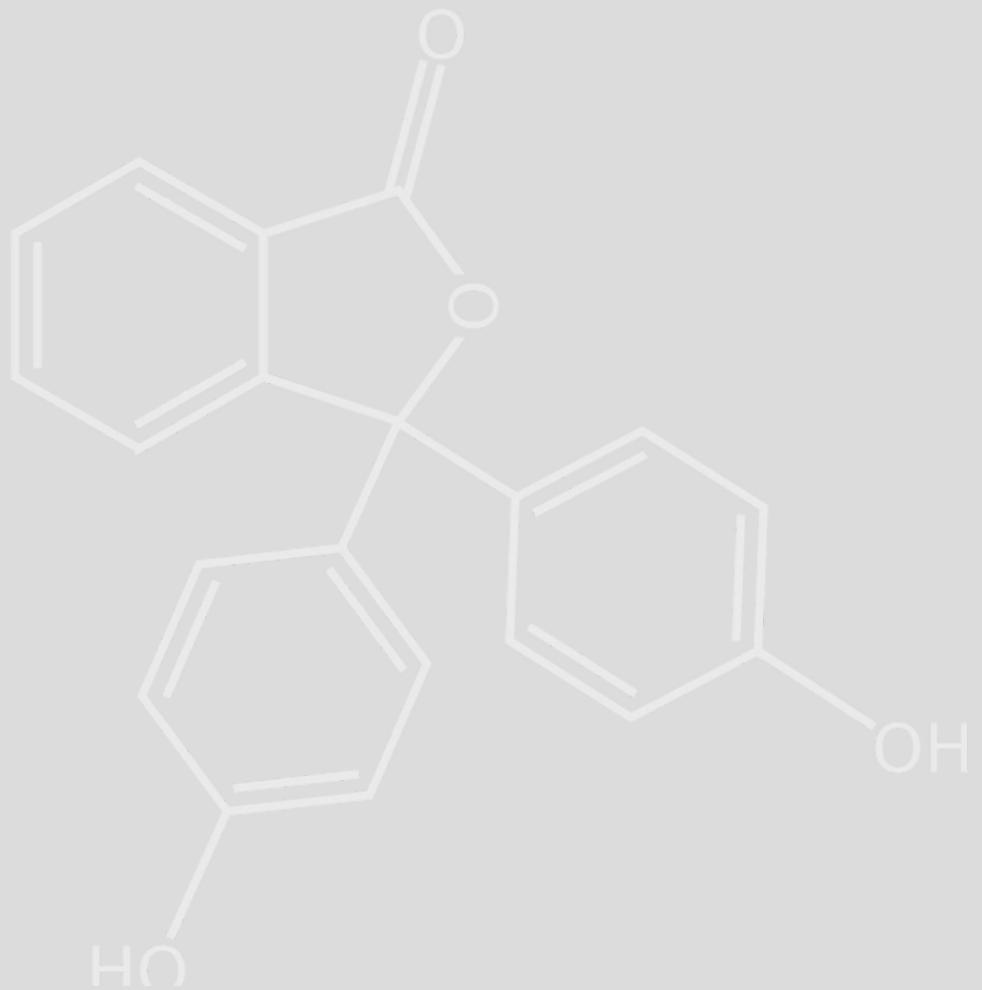


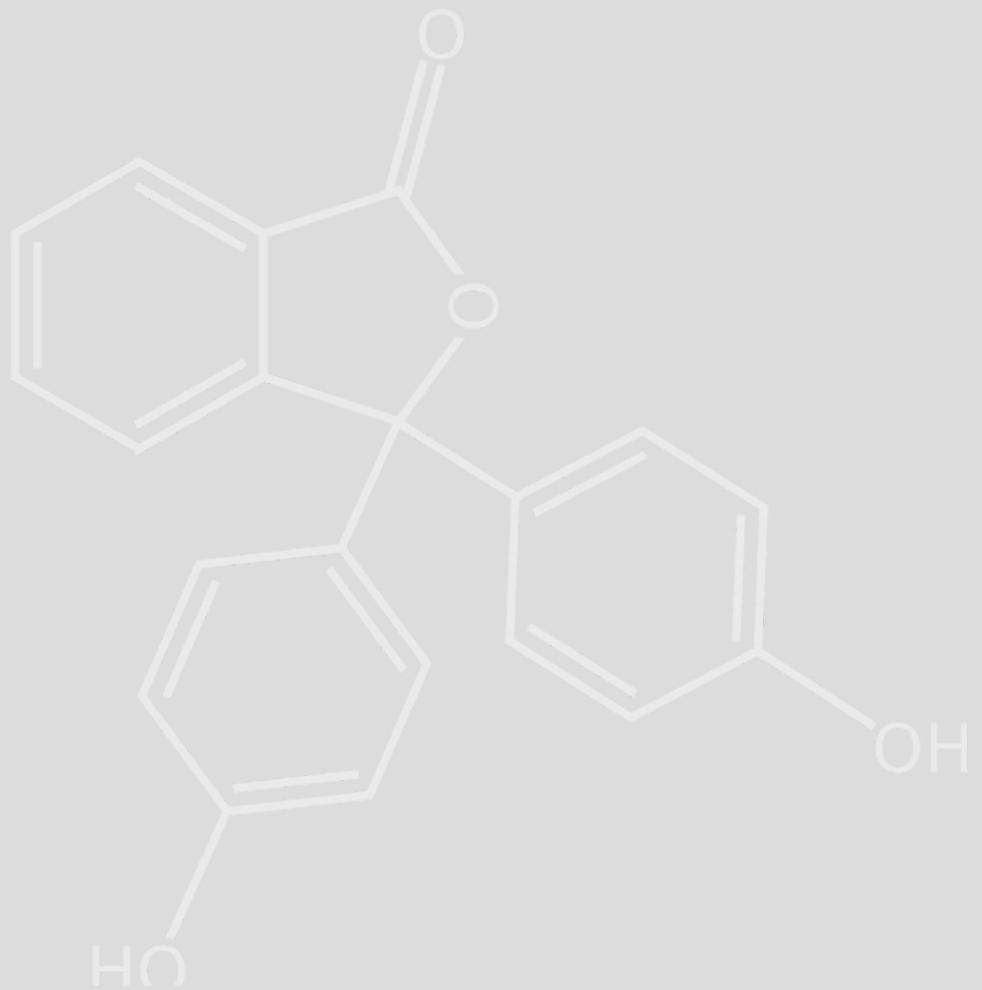


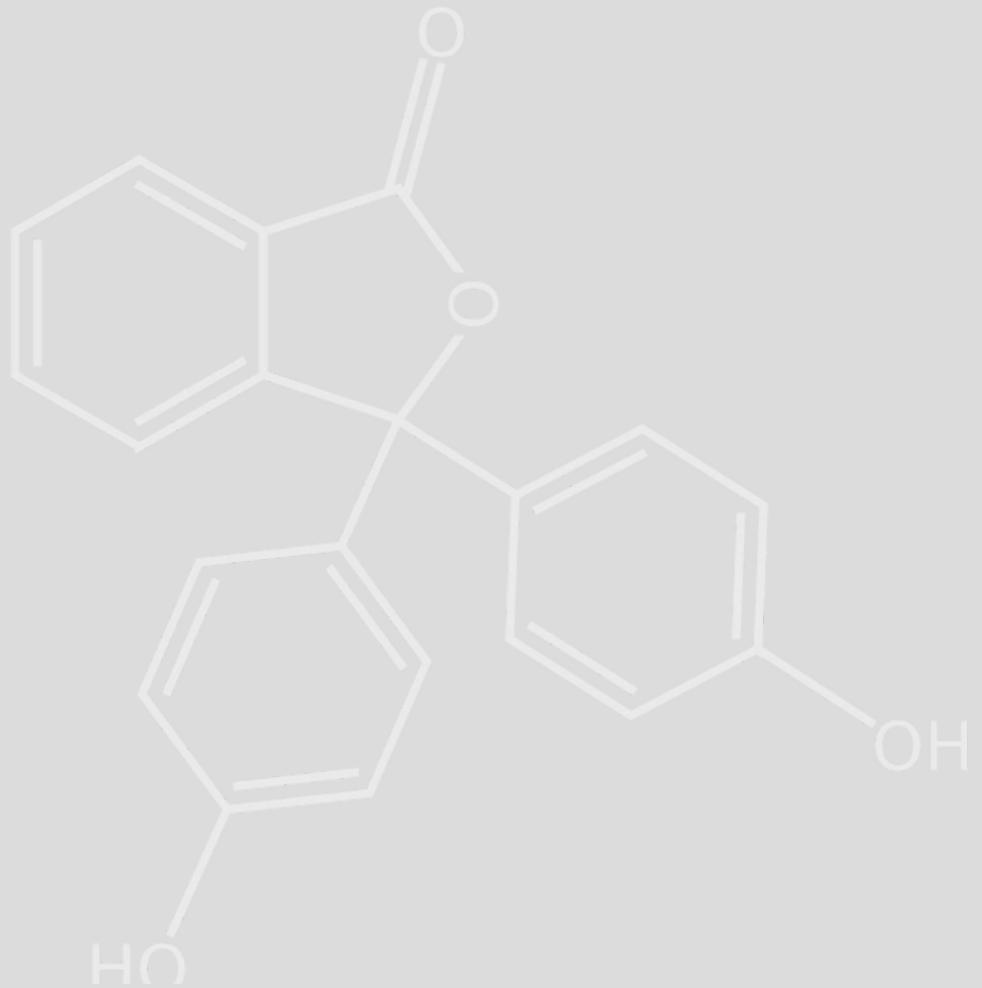


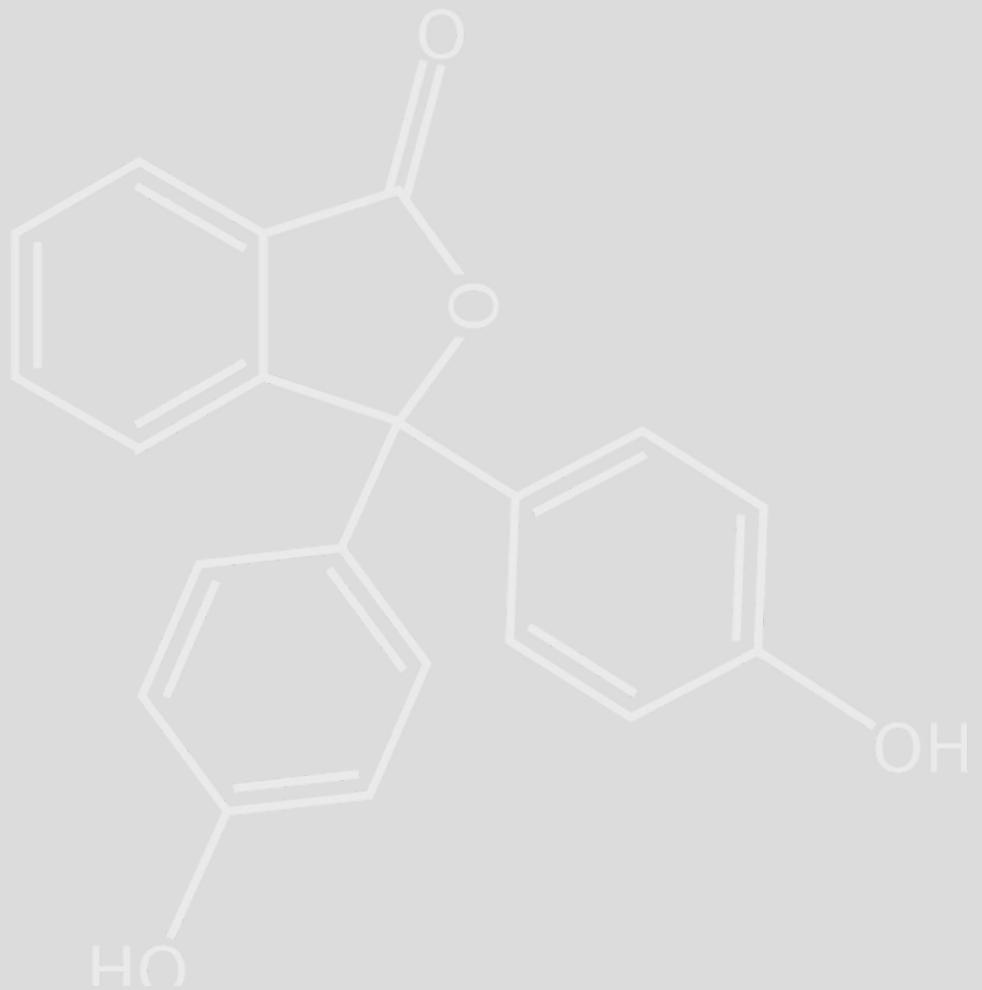


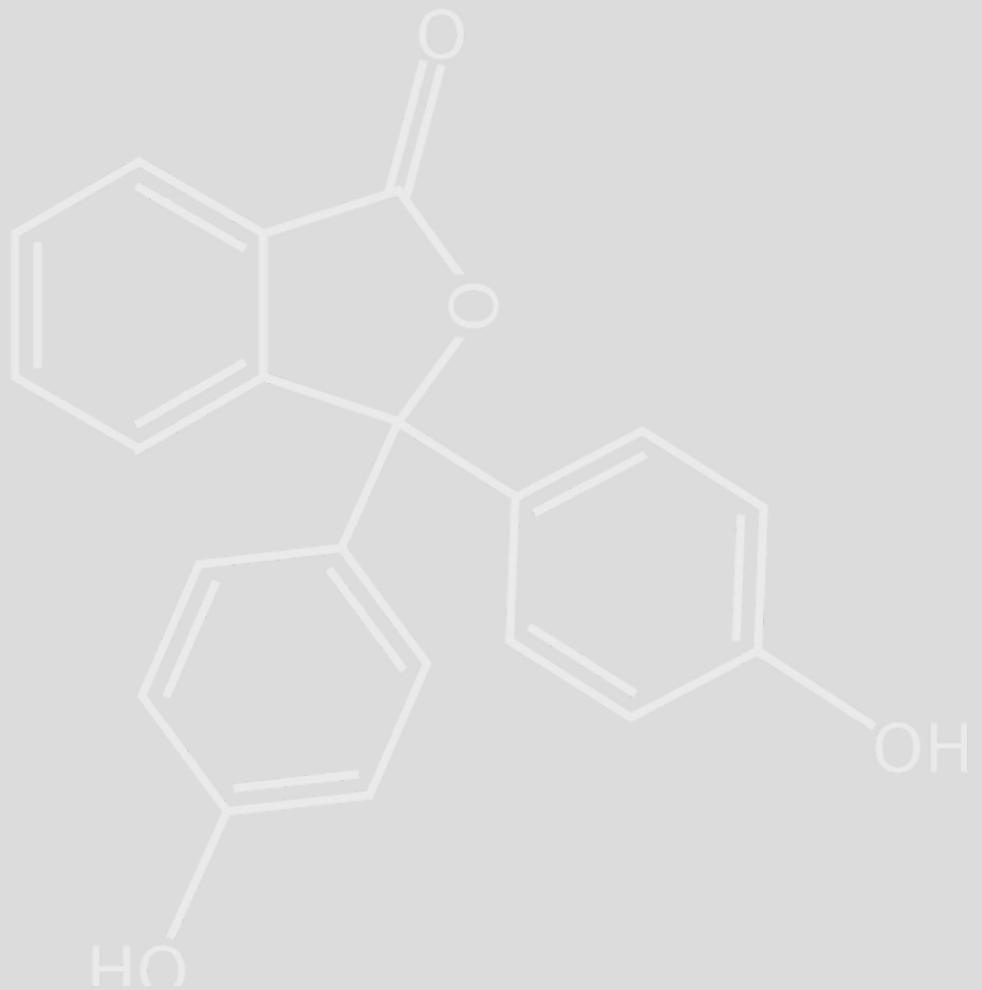


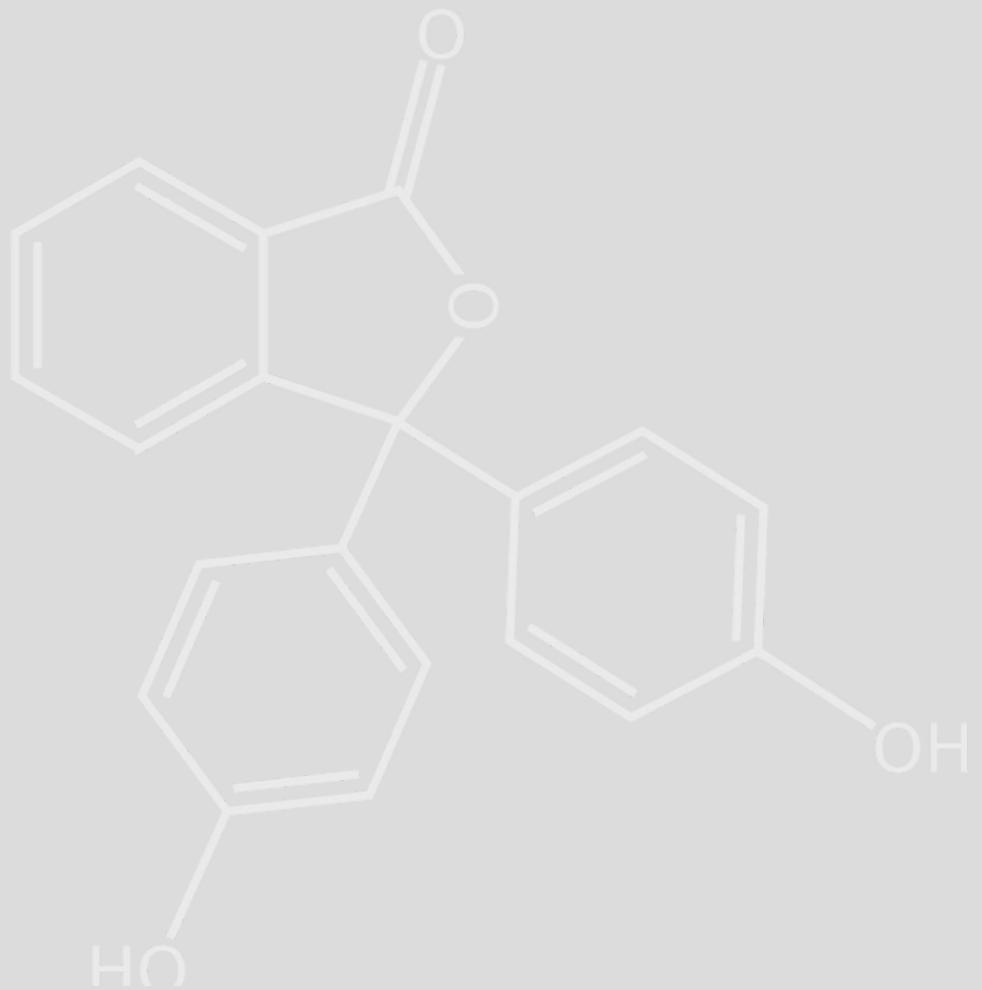


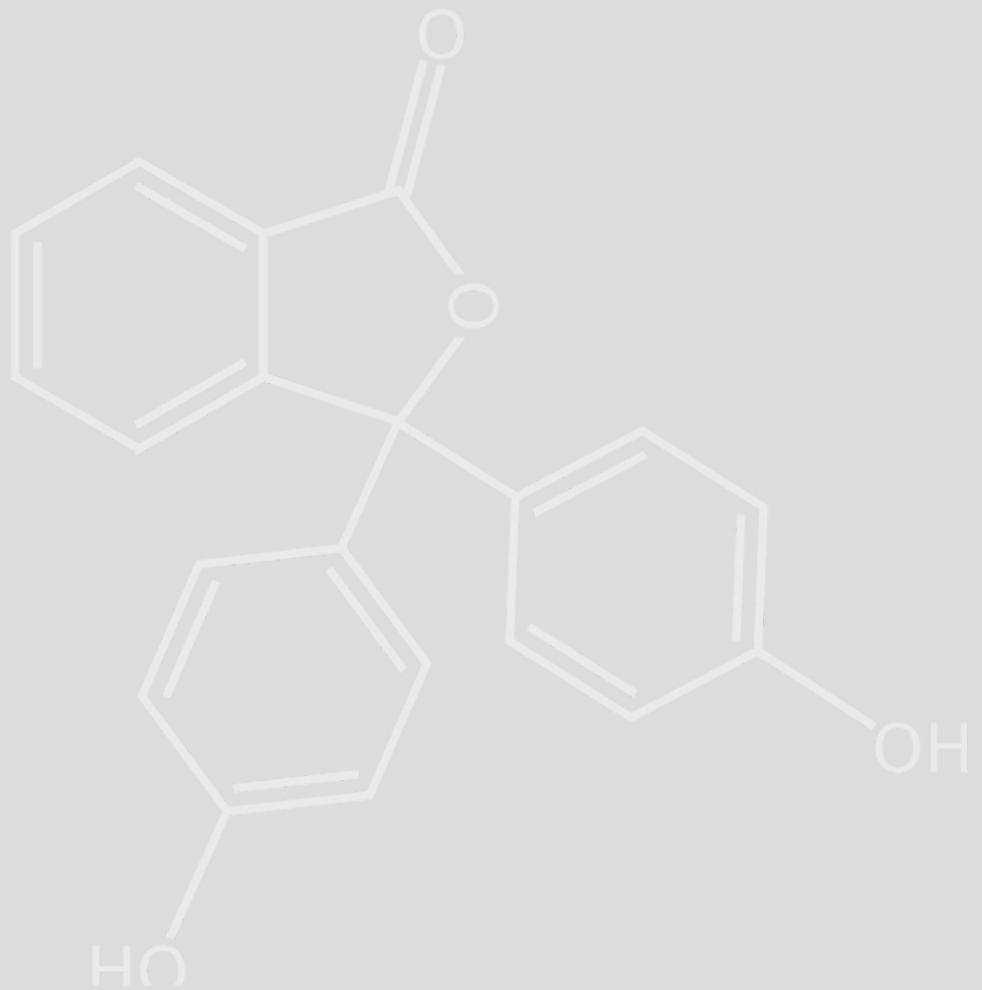


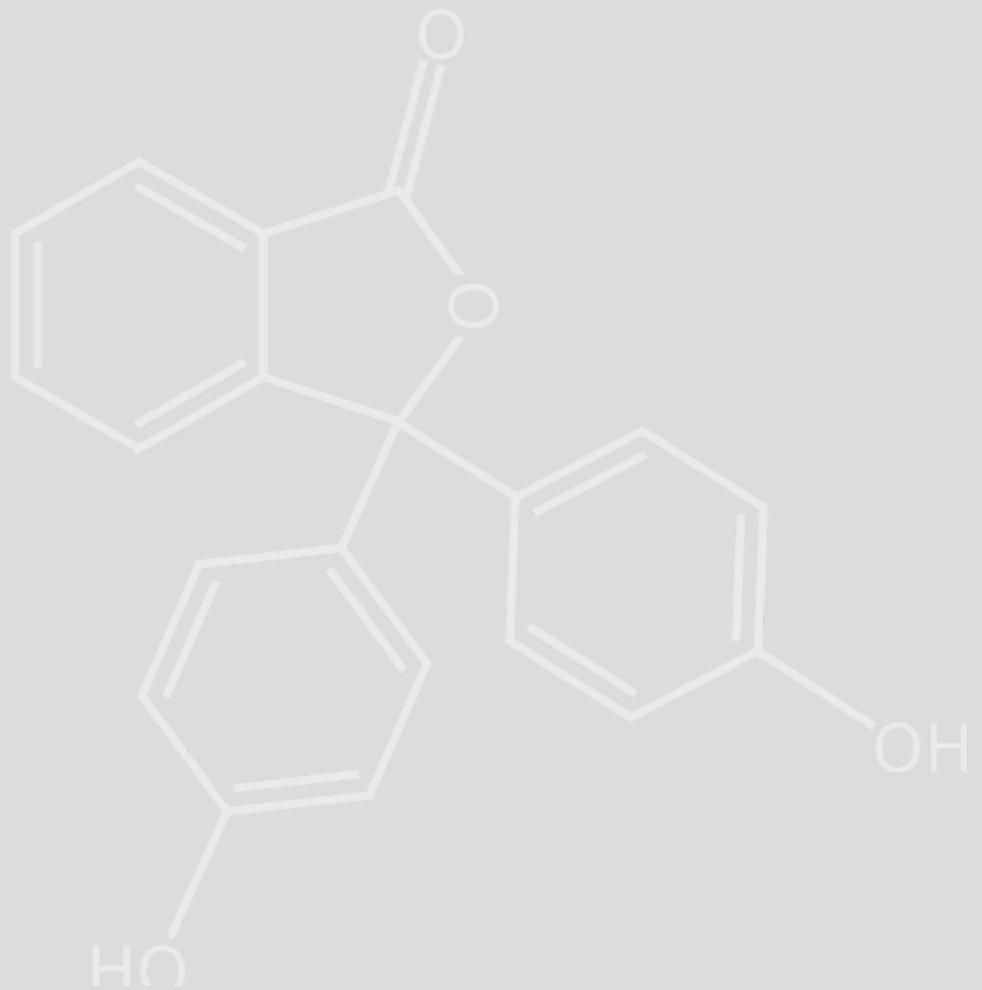


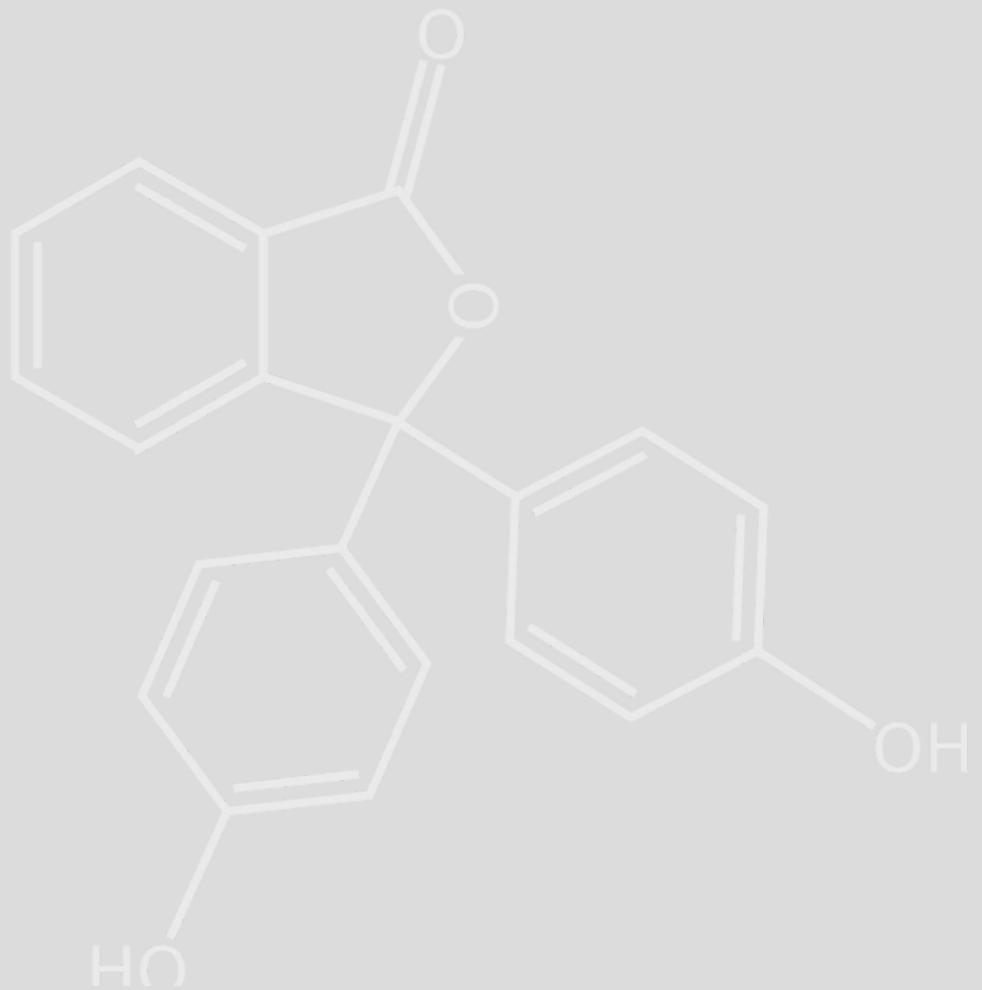


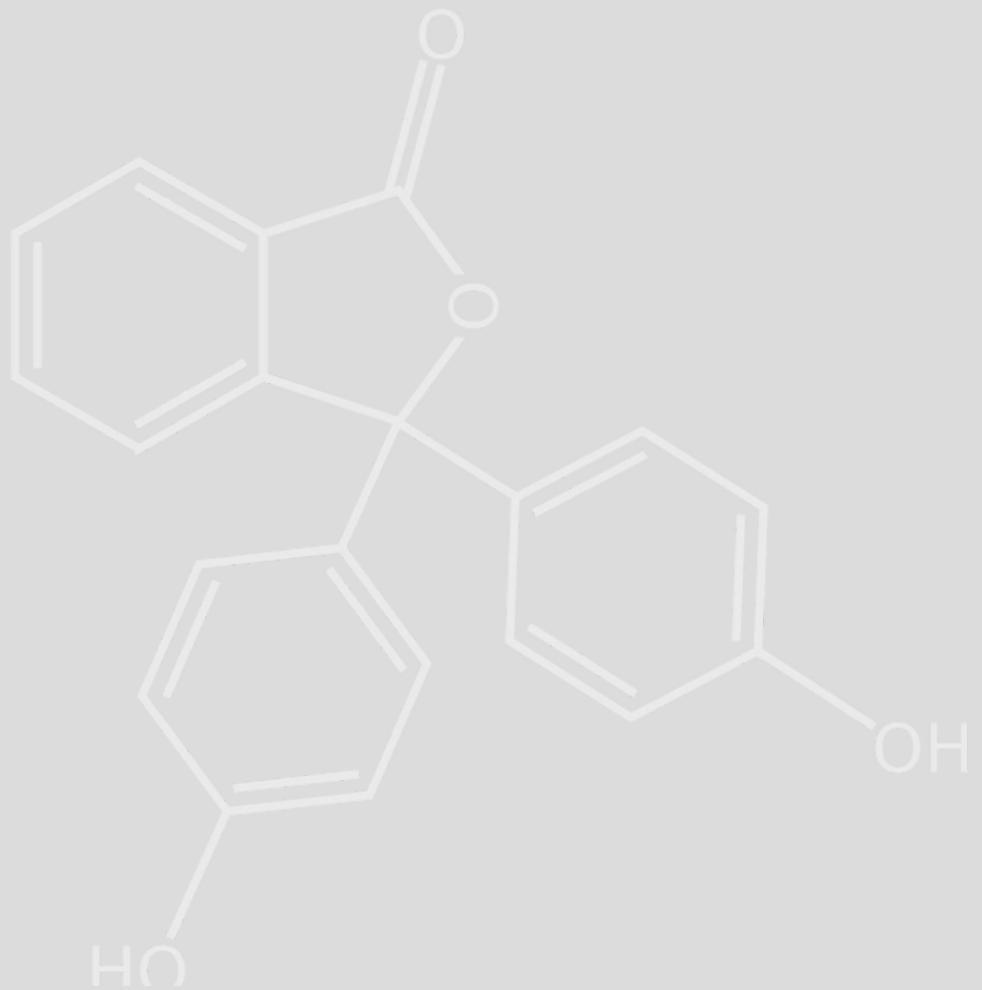


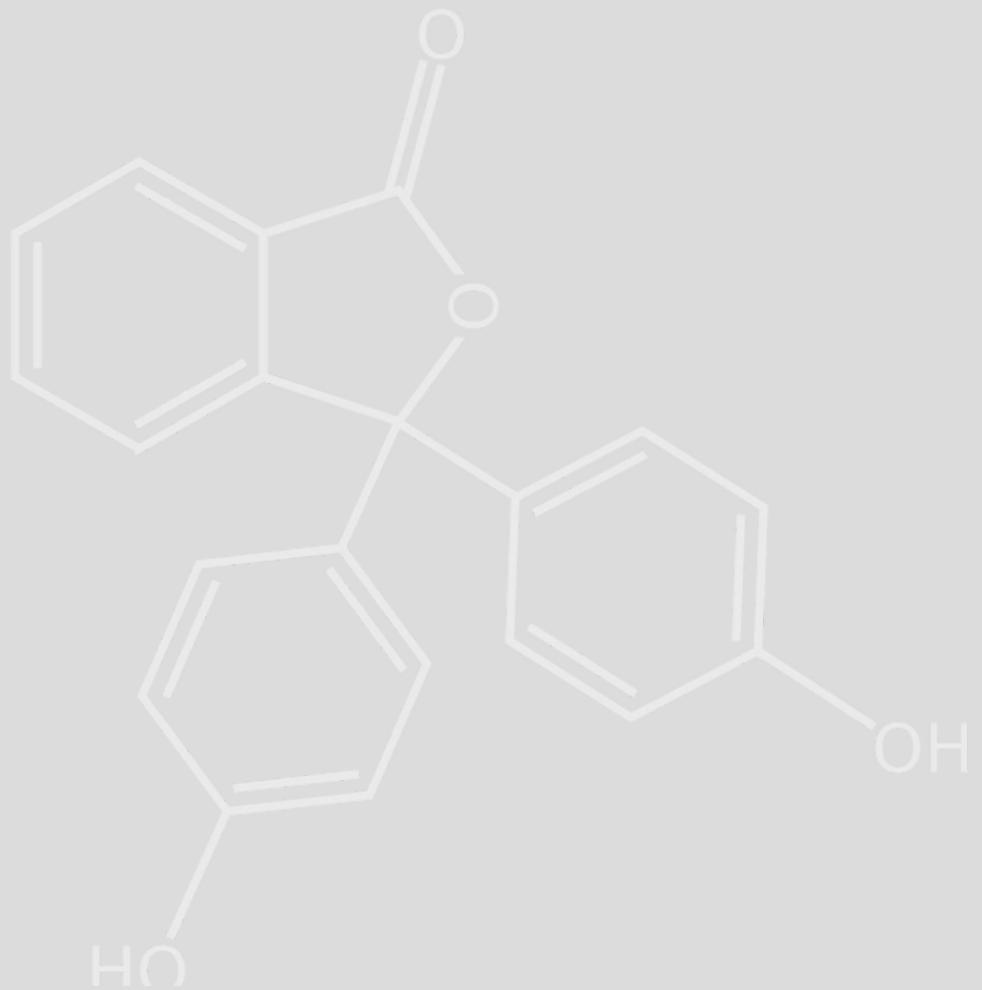


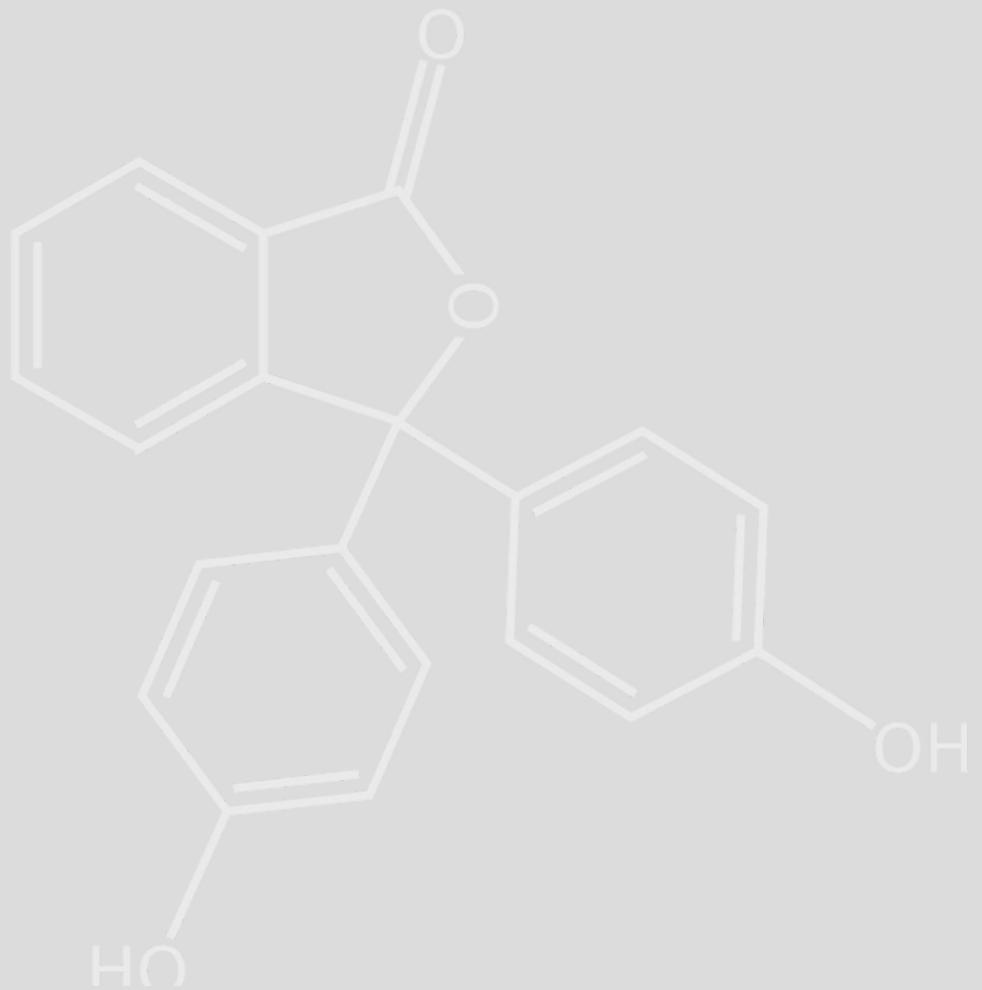


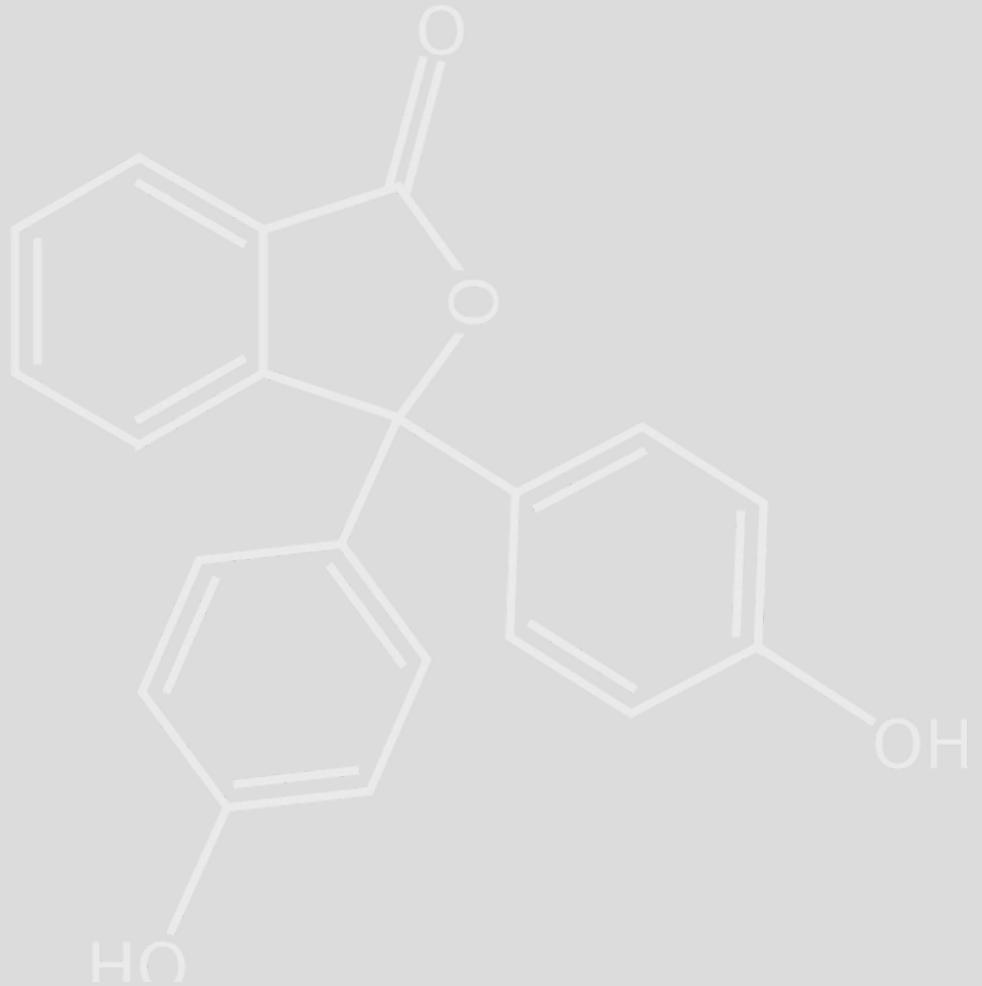


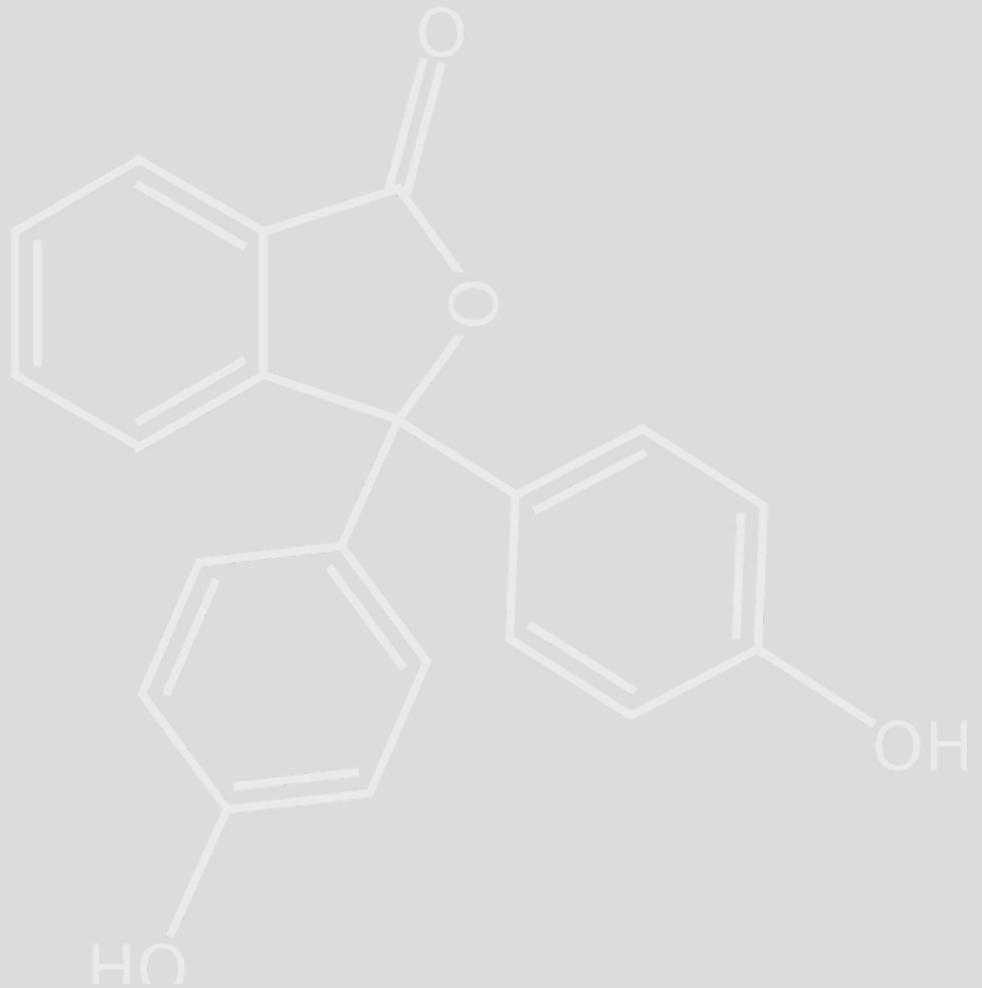


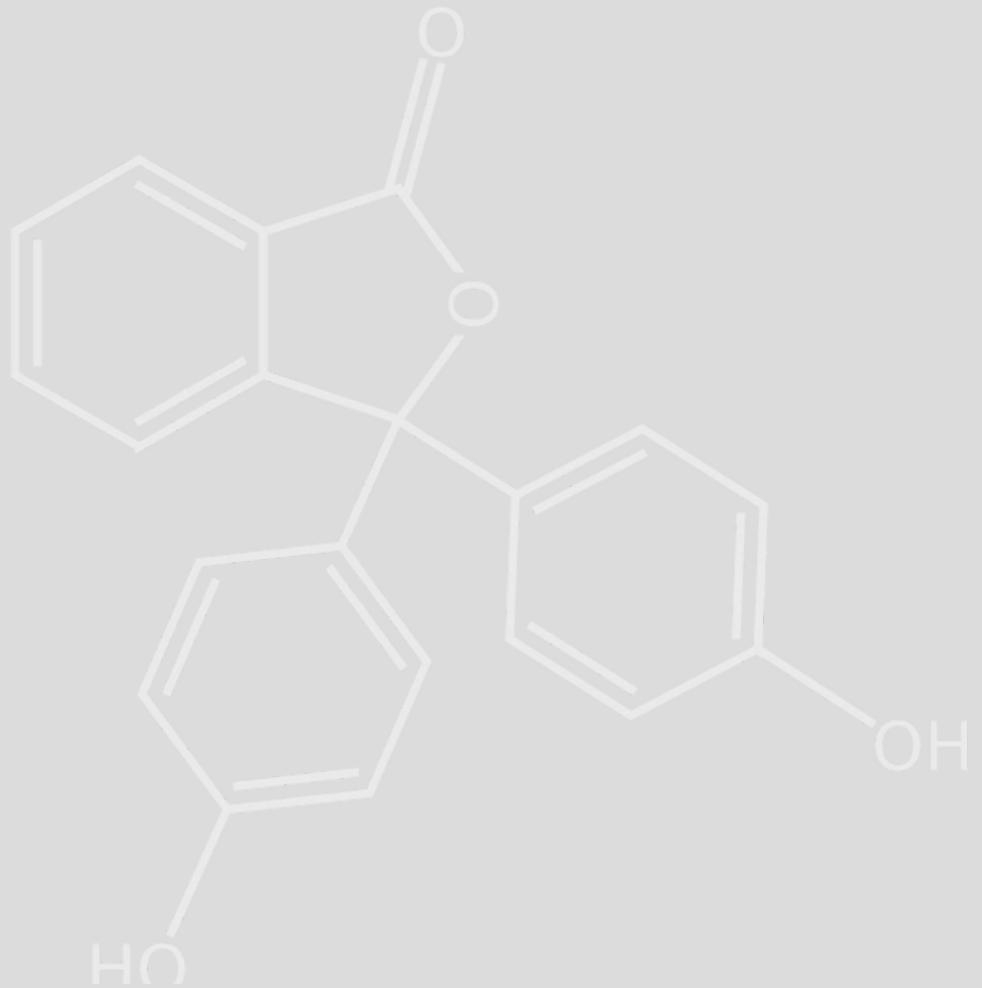


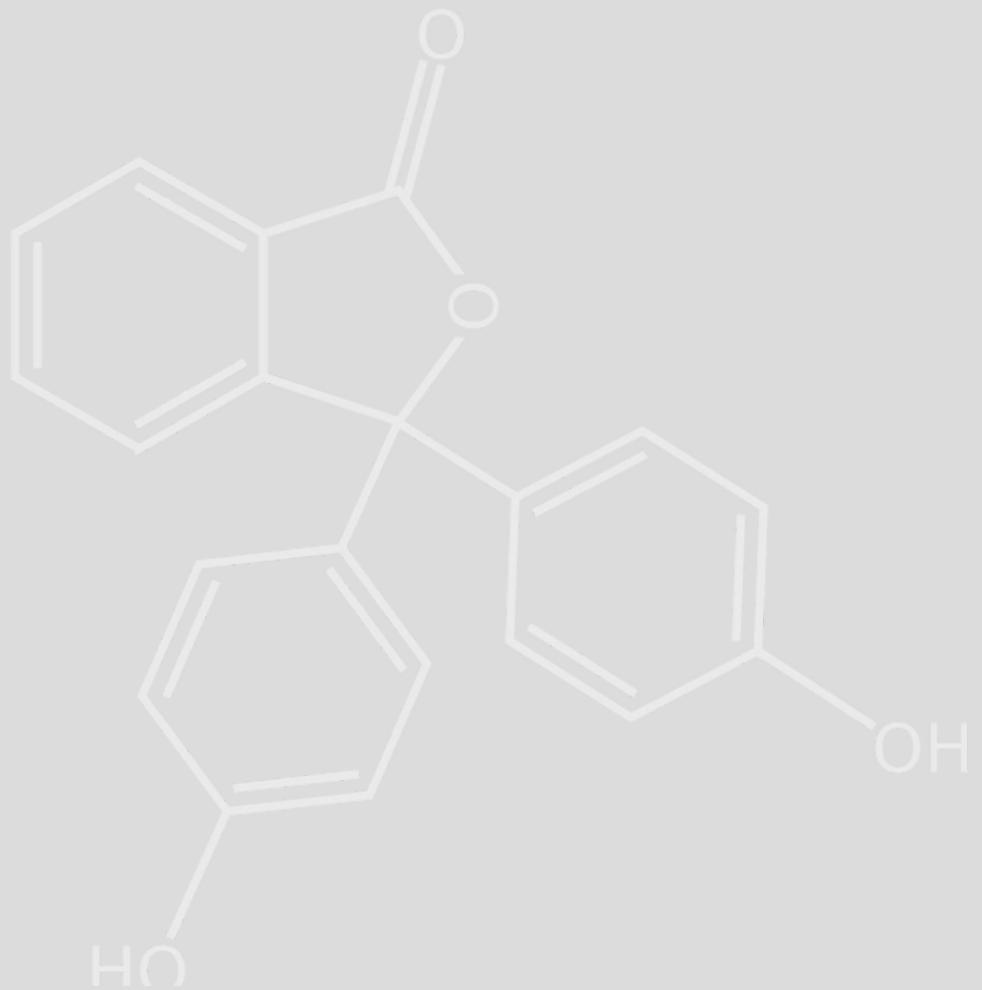


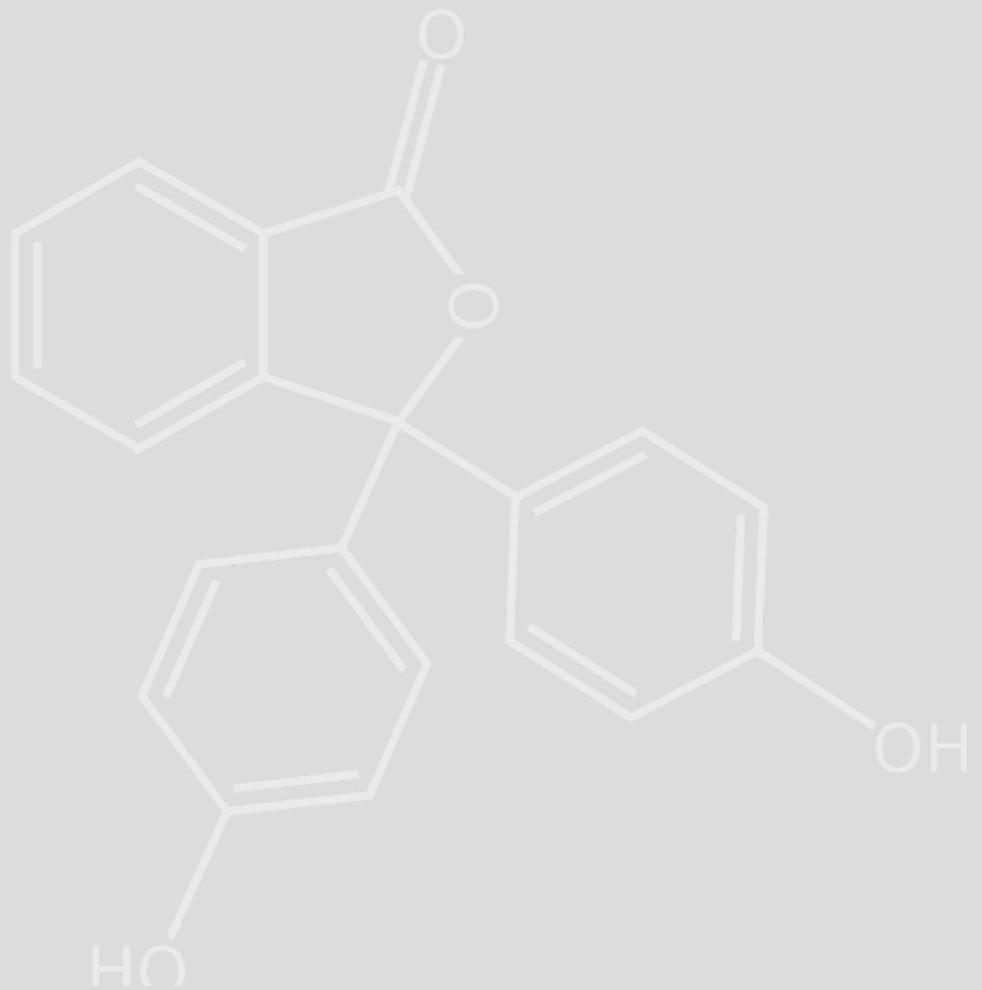


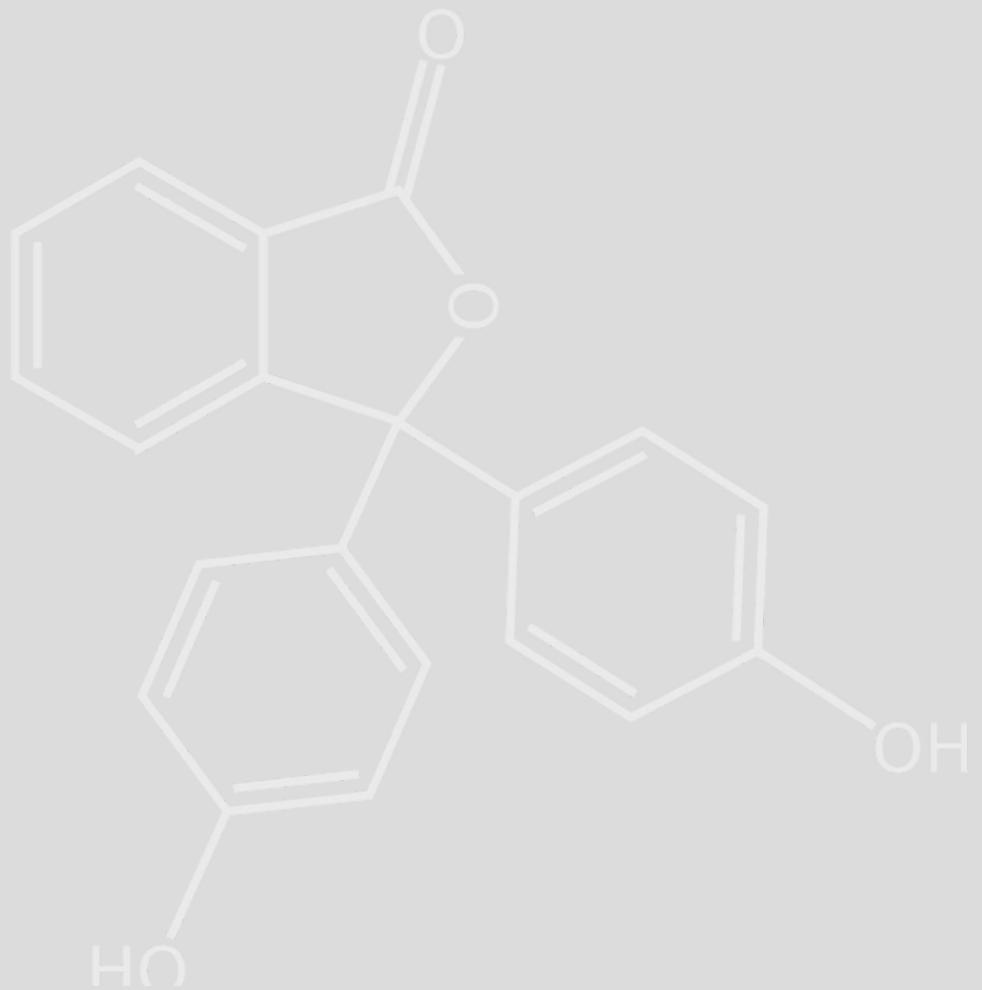


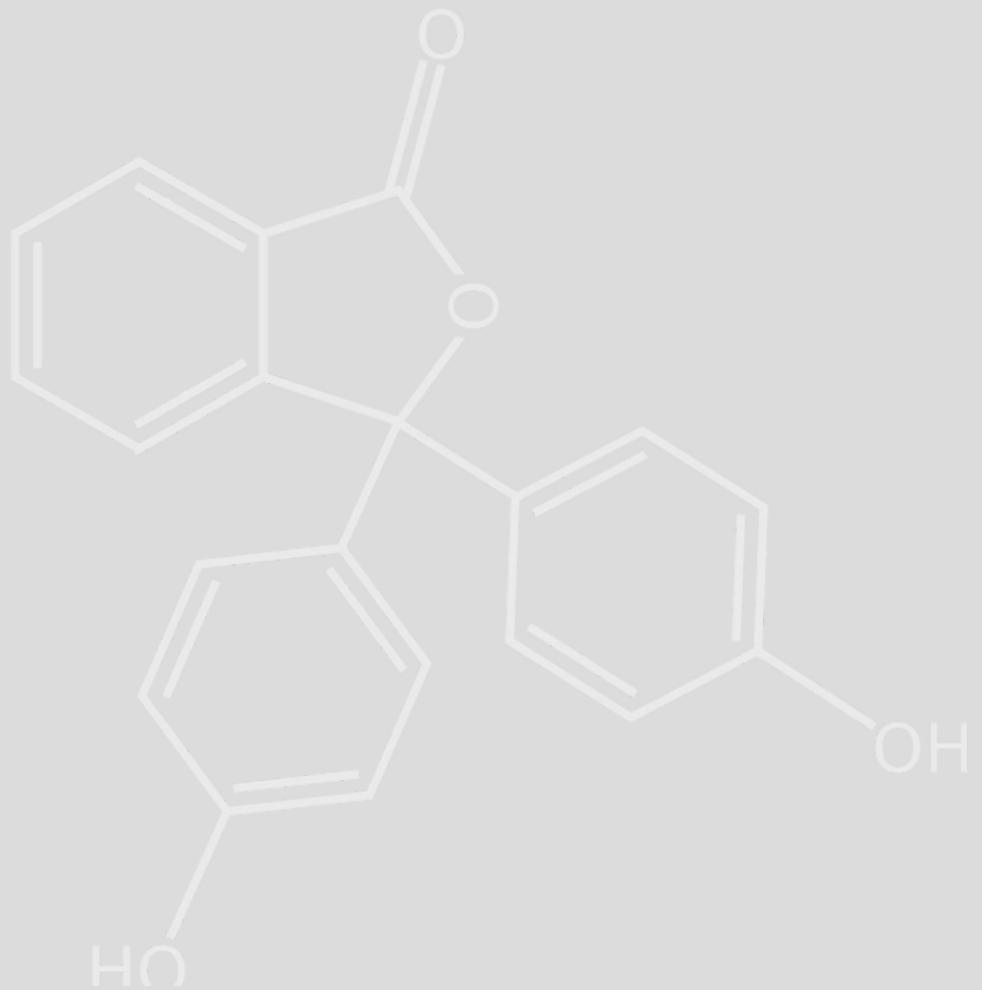


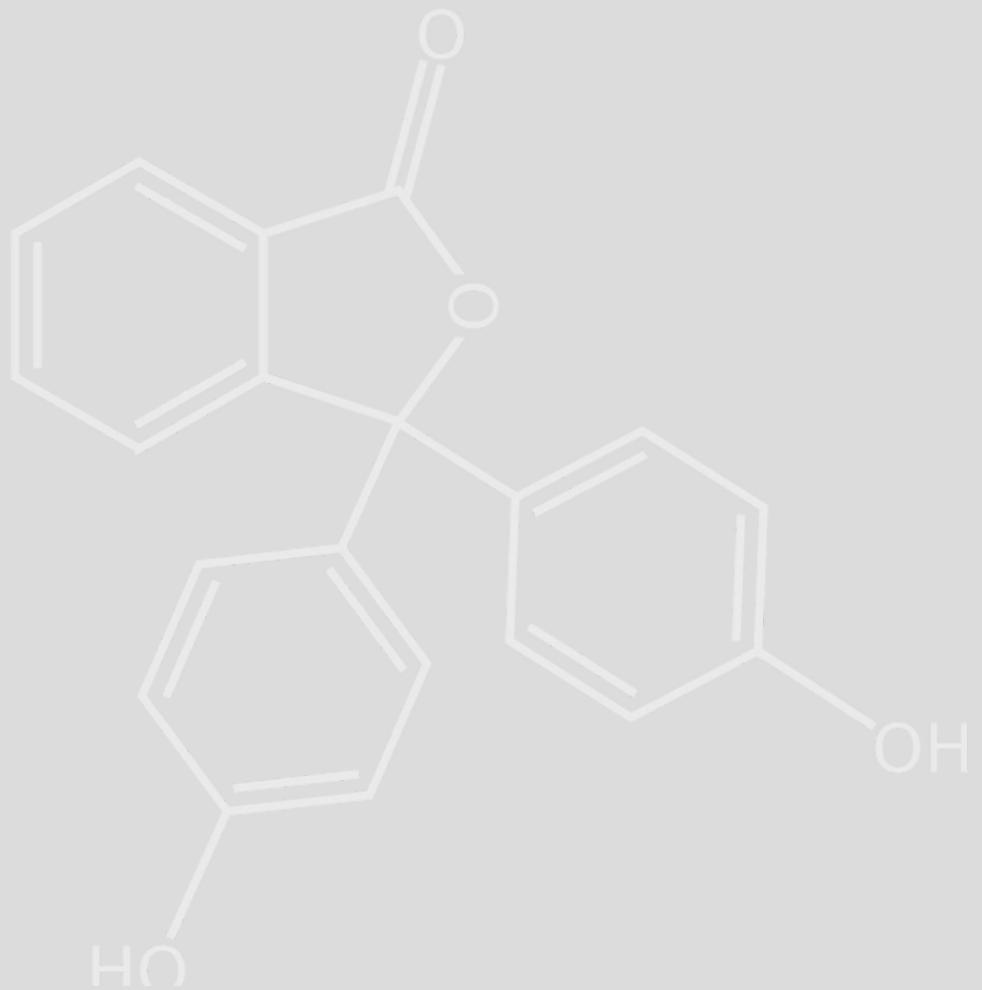


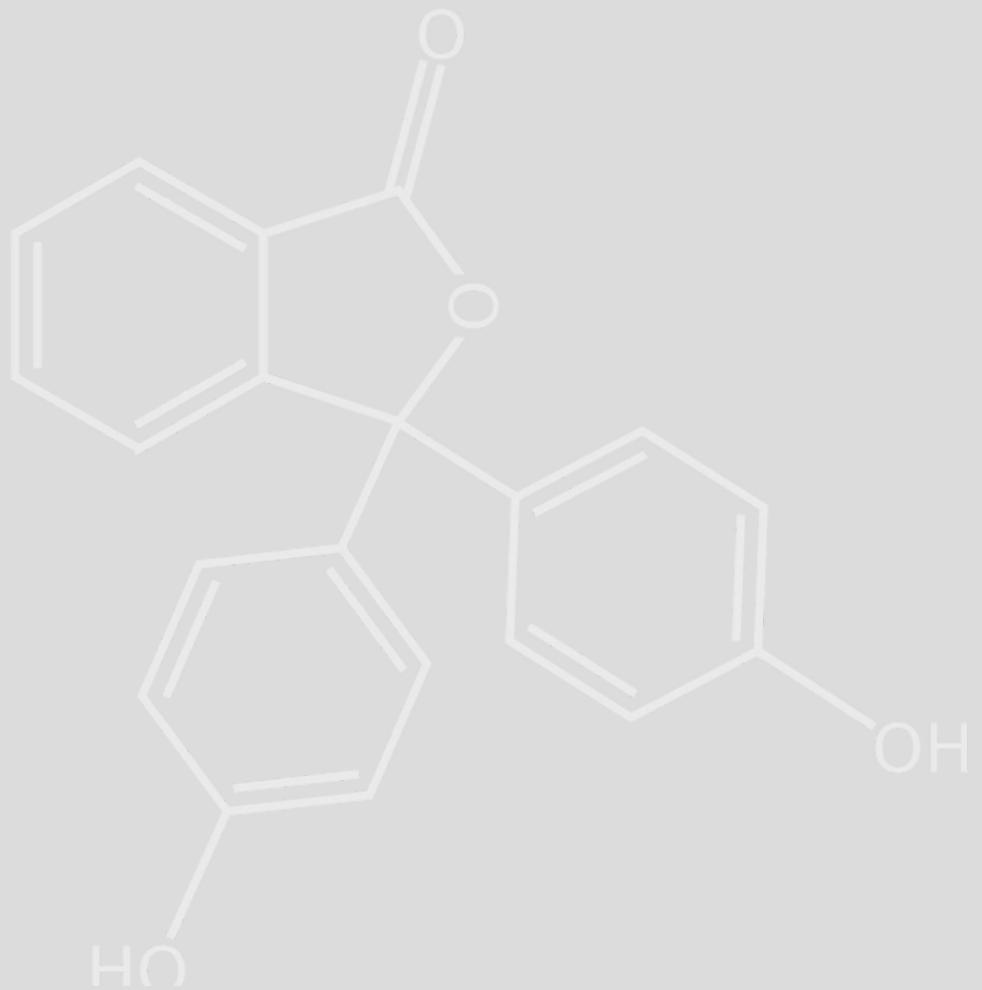


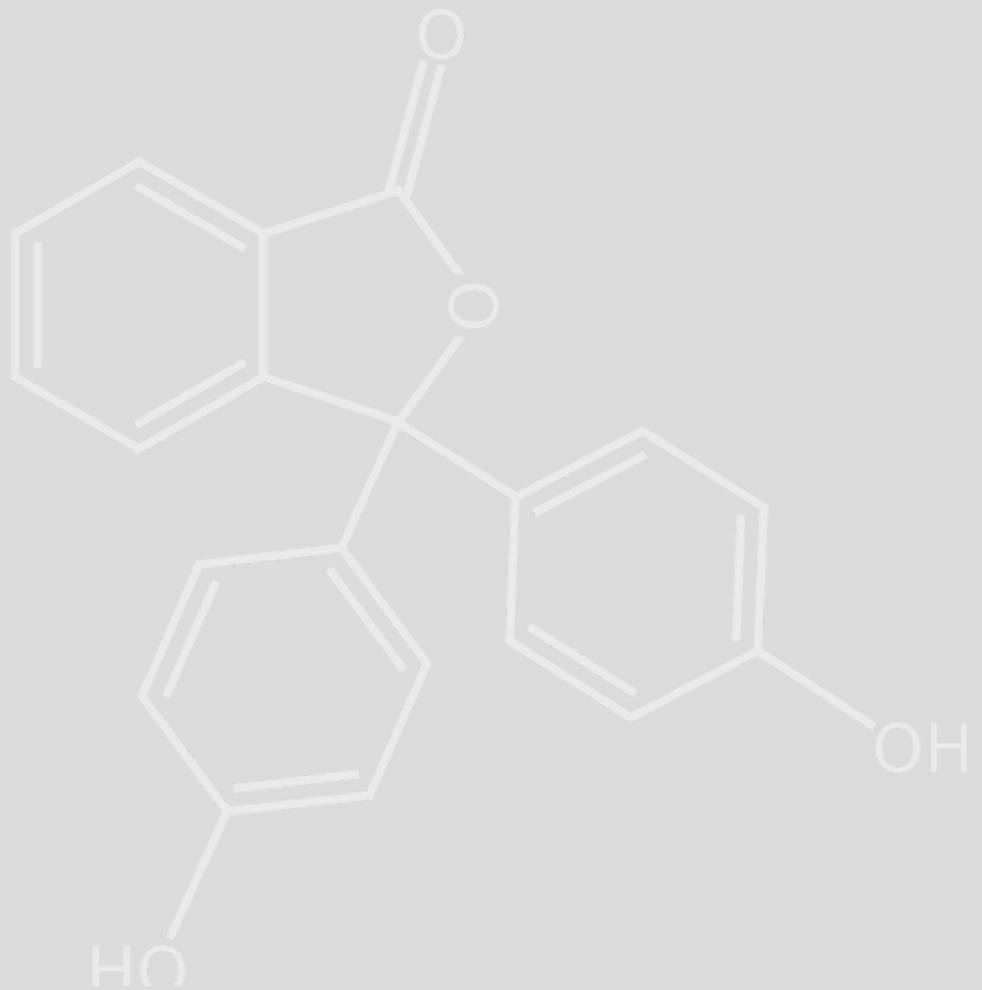


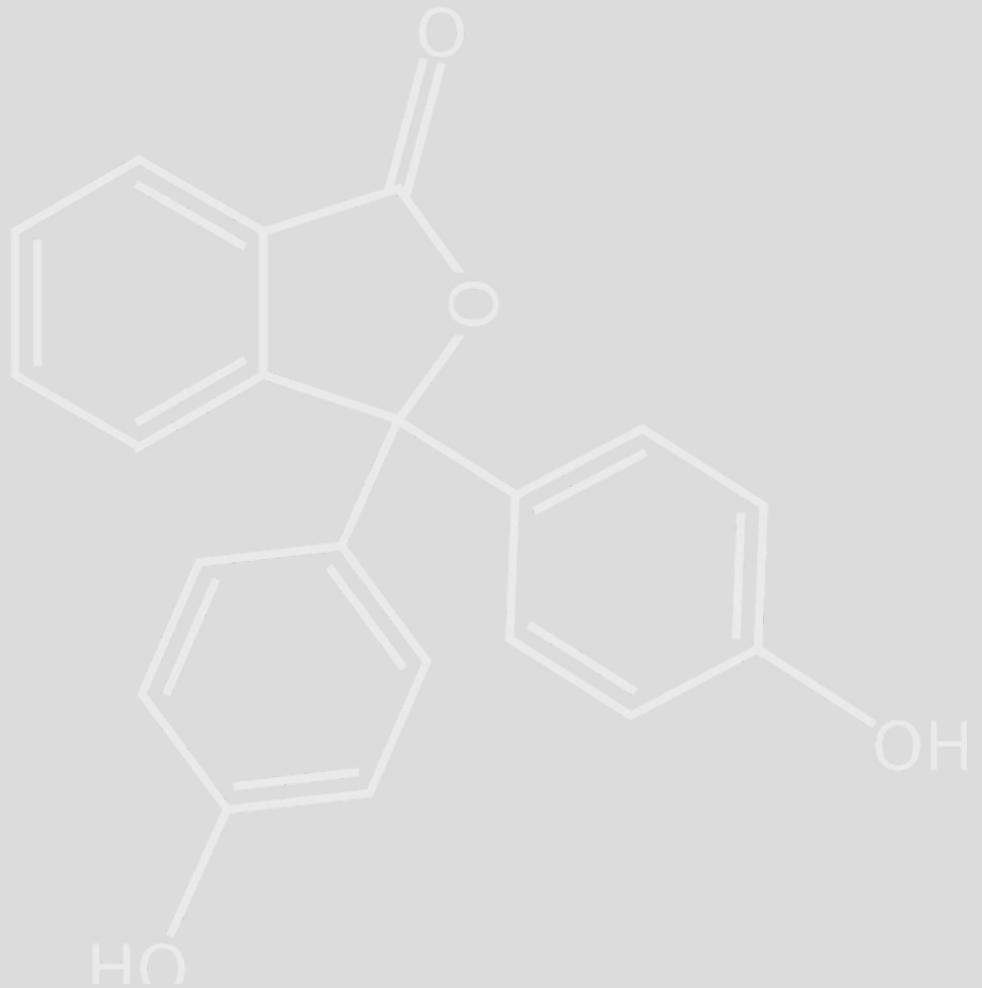


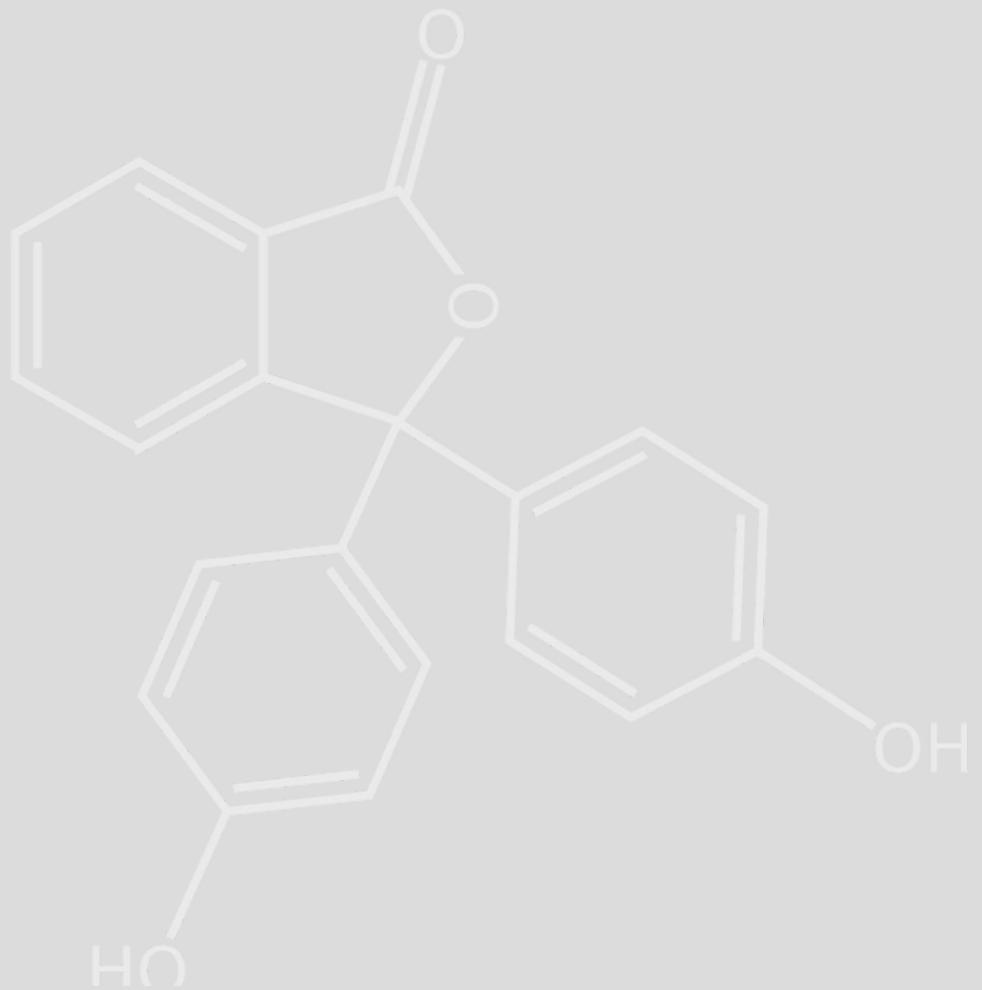


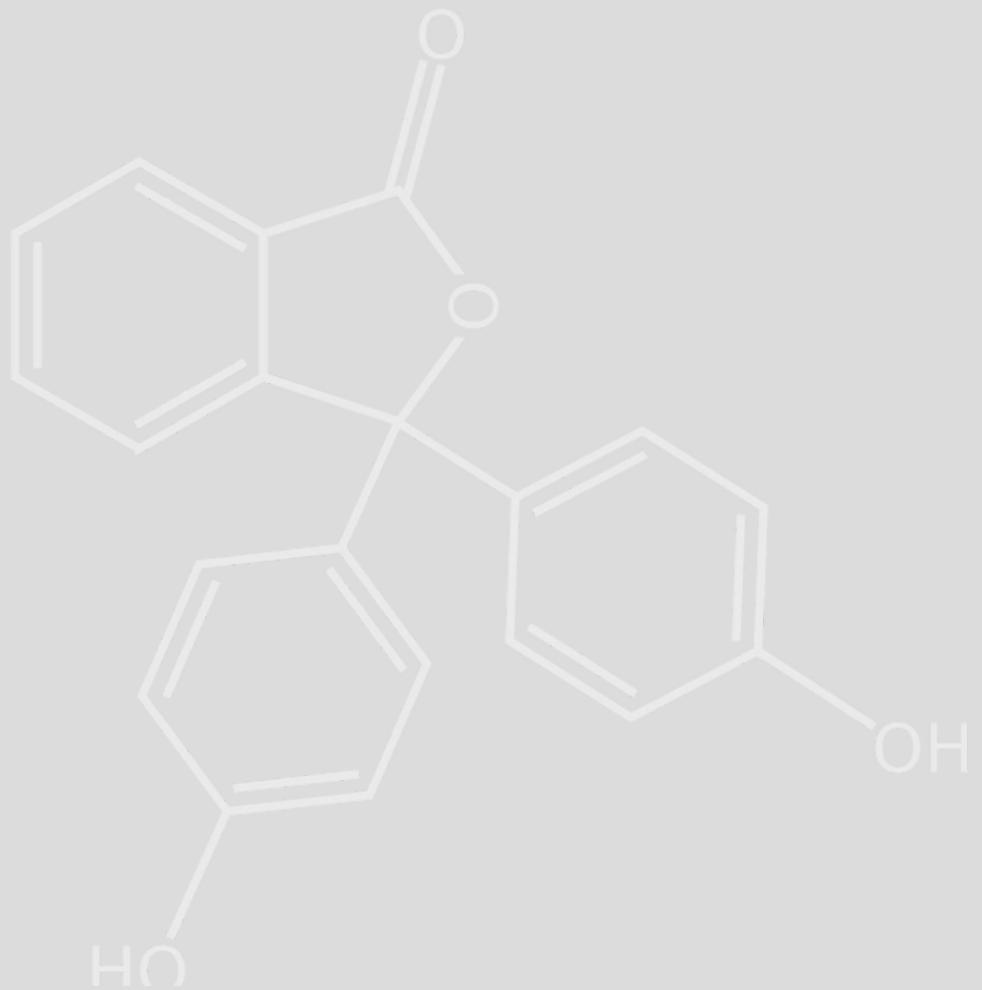


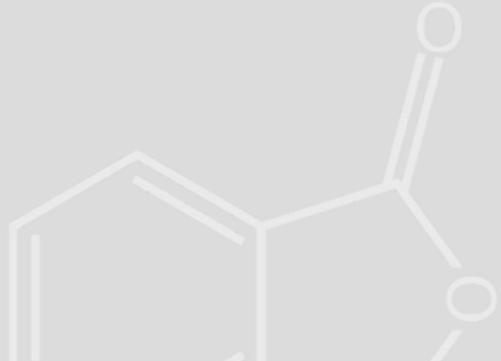












Having learned DFT, let us move to learning program packages. We begin by learning Quantum Espresso



The University of Tokyo

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