SYNTHESIS AND BIOLOGICAL EVALUATION OF SOME AZO DYES BASED ON 3-CYANO-6-HYDROXY-4-METHYL-1-PROPYL-2-PYRIDONE

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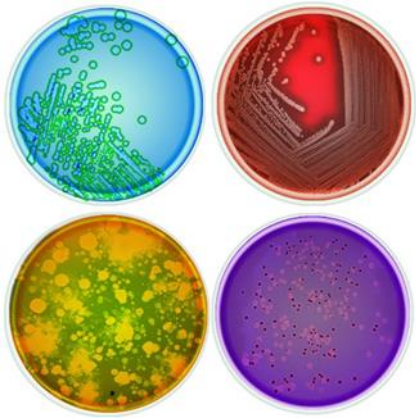
Heterocyclic azo dyes

- Excellent coloration properties
- Photovoltaics
- Pharmaceuticals
- More stable, brighter and ecologically acceptable then simple azo dyes

➢ Azo dyes based on 2-pyridone scaffolds:

- Cytotoxic activity
- Antibacterial properties
- Strong antioxidants (–OH and –NH groups)



Our work

- **Synthesis**:
- Three azo dyes have been synthesized from different aminophenoles and 3-cyano-6-hydroxy-4-methyl-2-pyridone

- **Structural characterization**:
- ATR-FTIR, NMR and UV-Vis analysis

- **Biological evaluation**:
- *In vitro* antioxidant activity by ATBS method
- *In silico* evaluation of physico-chemical parameters and ADME (absorption, distribution, metabolism, and excretion) properties by SwissADME

Synthesis

- **Diazo-coupling reaction**
- Diazo components:

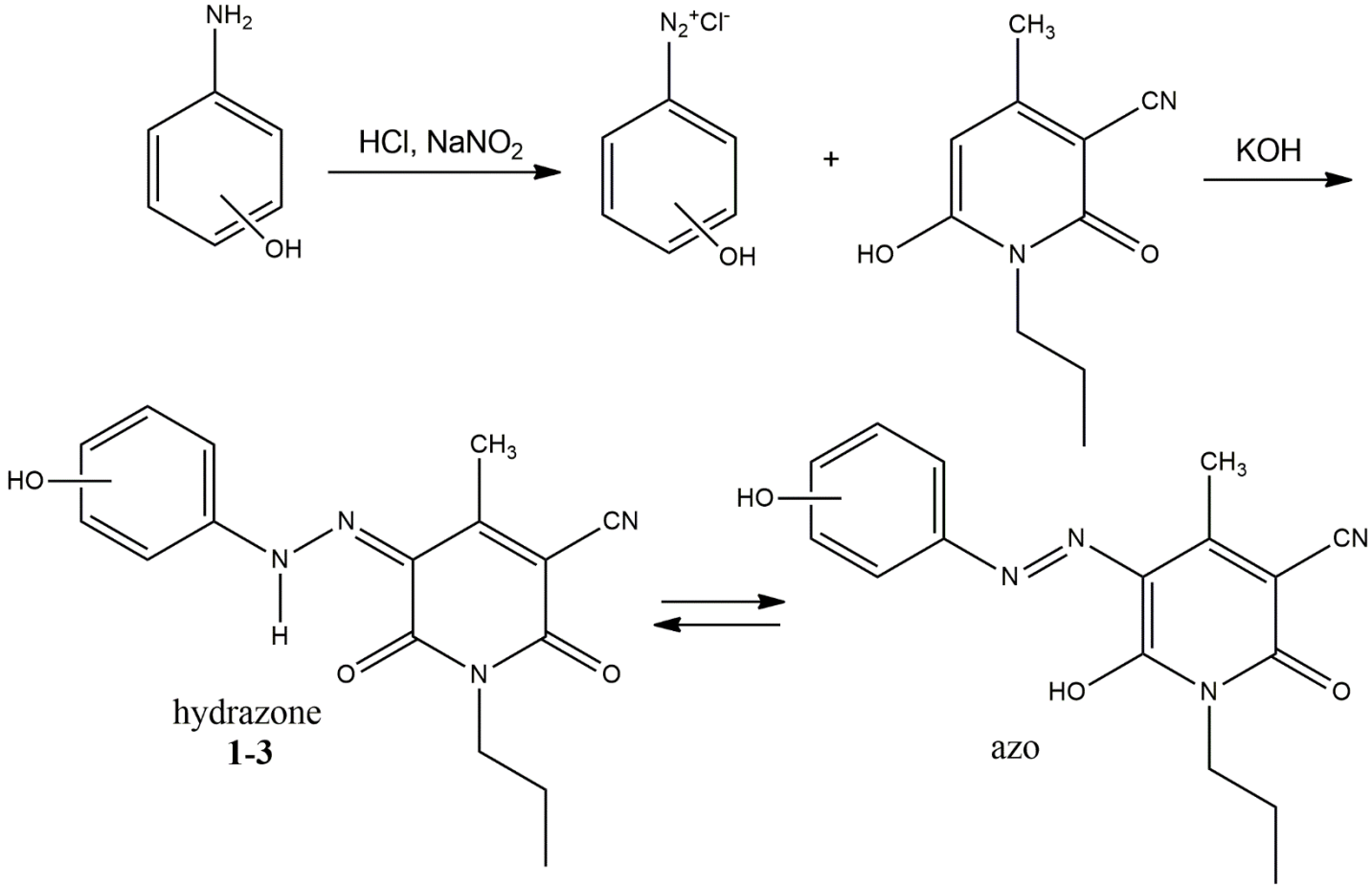
2-aminophenol (1)

3-aminophenol (2)

4-aminophenol (3)

- Coupling component:

3-cyano-6-hydroxy-4-methyl-1-propyl-2-pyridone



Structural characterization

ATR-FTIR

1667–1659 and 1625-1621 cm^{-1} (C=O)

3367–3213 cm^{-1} (N–H)

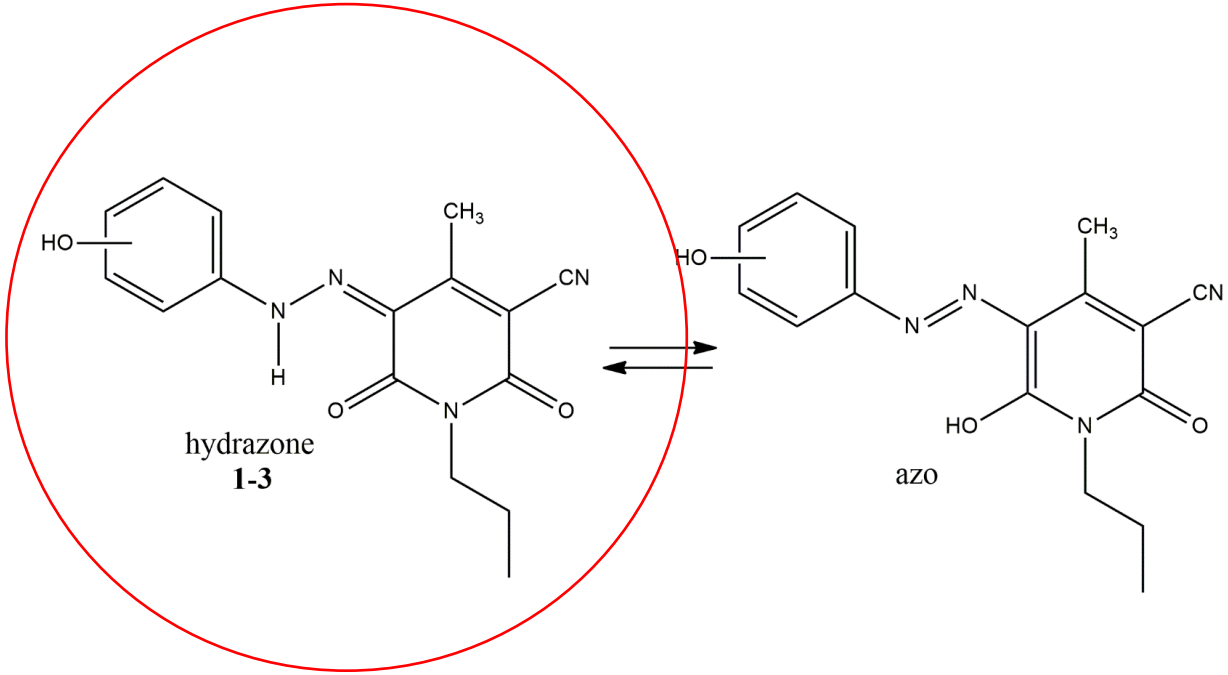
1509–1501 cm^{-1} (C=N and N–H)

NMR

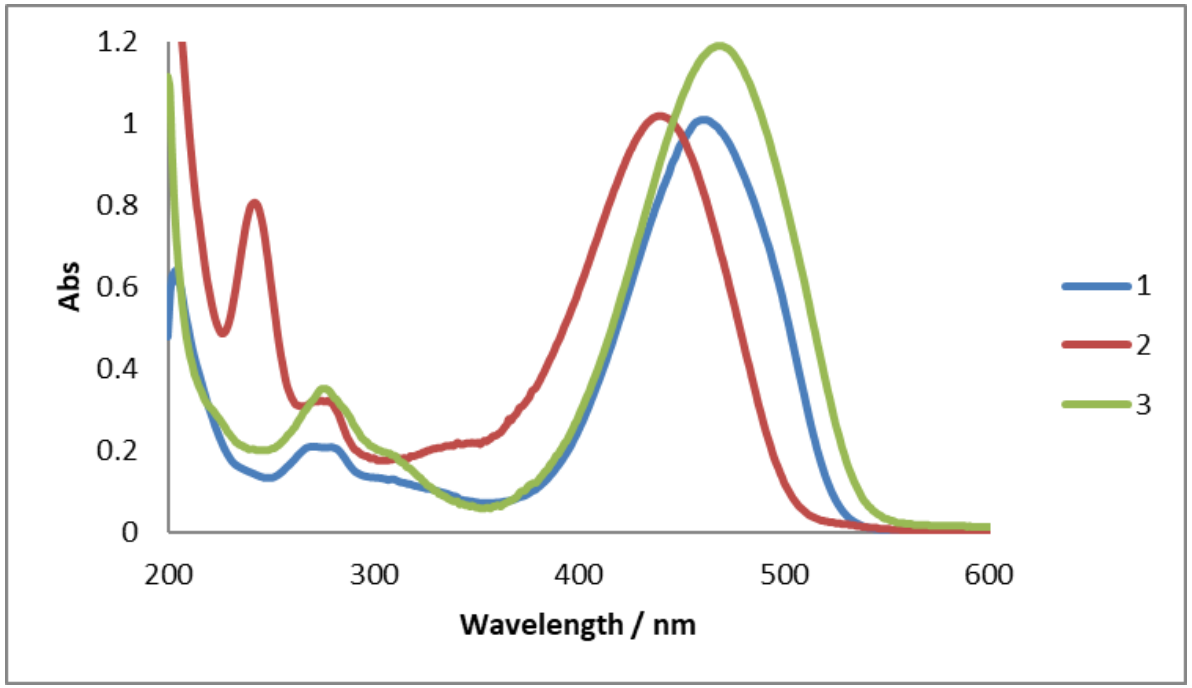
14.98–14.52 ppm (proton of the hydrazone N–H group)

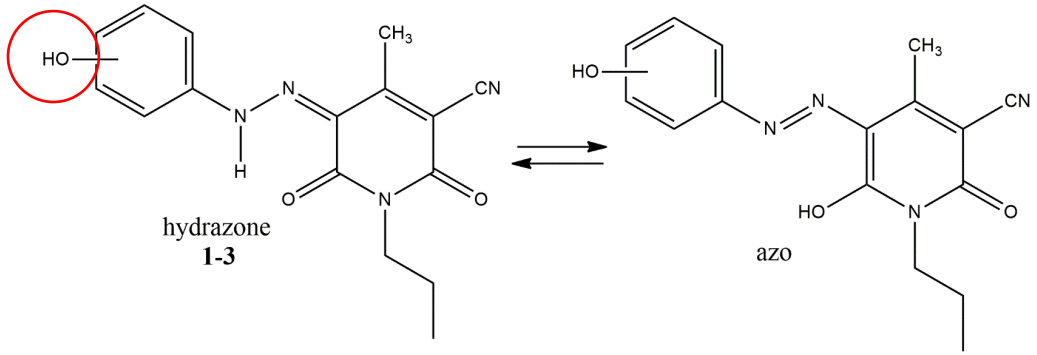
UV-Vis

λmax at 459.5 (**1**), 440.0 (**2**) and 465.8 (**3**) (π-π* transition between pyridone and phenyl moiety)



UV-Vis analysis





465.8 (**3**) > 459.5 (**1**) > 440.0 (**2**)

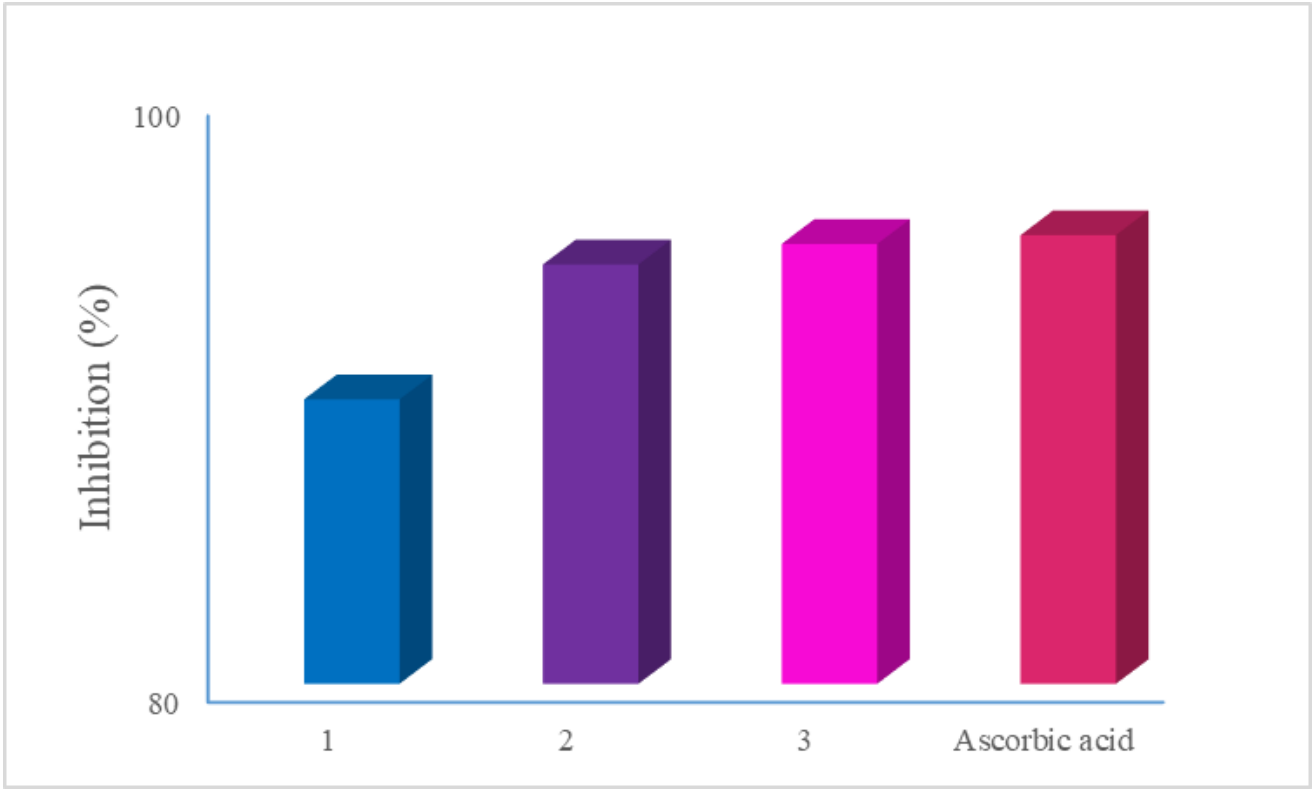
Biological evaluation

- **Antioxidant properties**

- Inhibition:

3 (95.0%) > **2** (94.3%) > **1** (89.7%)

- Excellent ability to scavenge the $ABTS^{\bullet+}$ radical cation comparing to the inhibition of ascorbic acid (95.3%)



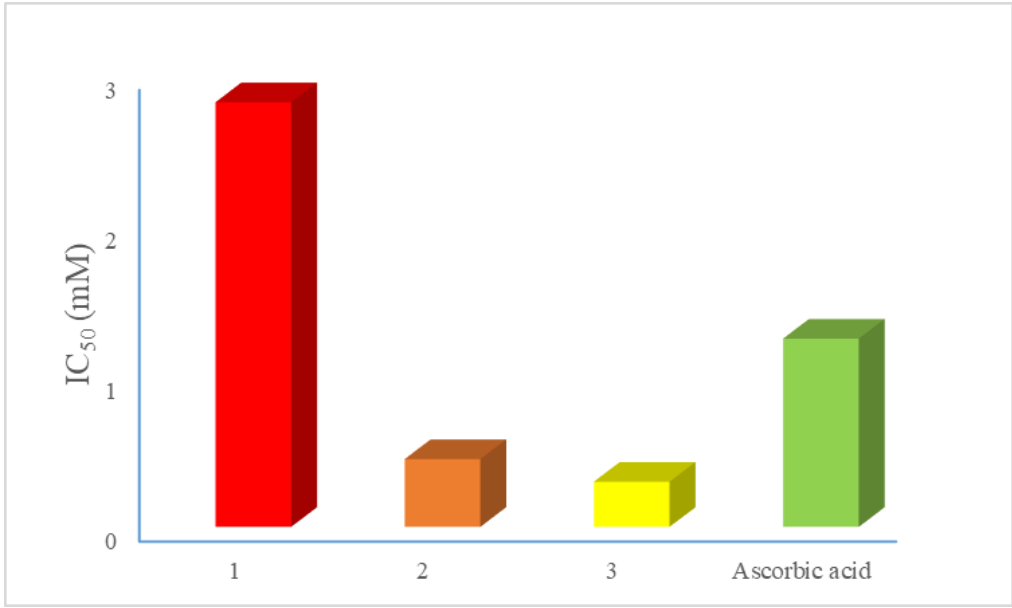
Biological evaluation

- **Further evaluation of antioxidant activity**

- **IC_{50} determination**

3 (0.3 mM) > **2** (0.45 mM) > **1** (2.80 mM)

IC_{50} of ascorbic acid 1.25 mM



Biological evaluation

- ***In silico* evaluation of physicochemical and ADME properties**

Dye	HBD	HBA	M log P	MW	Lipinski's violations	TPSA [Å²]	%ABS	Rot. Bond
1-3	2	5	0.76	312.32	0	105.79	72.50	4

All investigated compounds may be orally bioavailable with no permeation to the blood brain barrier.

Thank you for your attention!