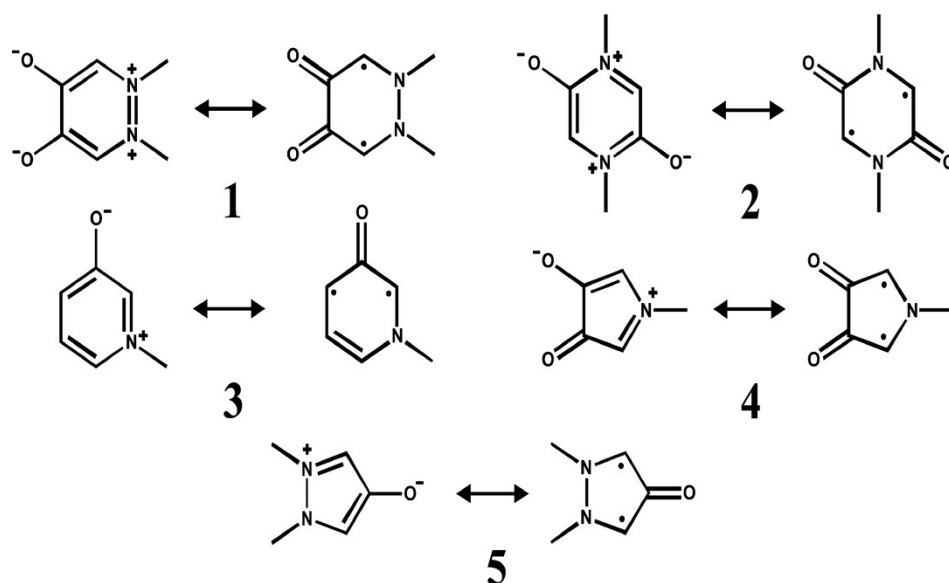




**Figure S1** List of five other compounds predicted for the future study. Numeber **2** was used in this paper.

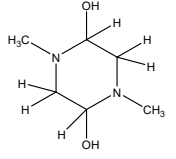
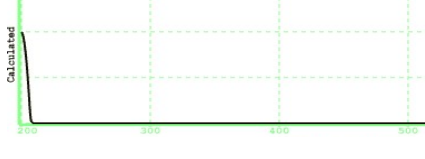
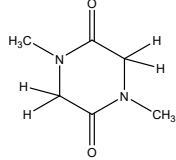
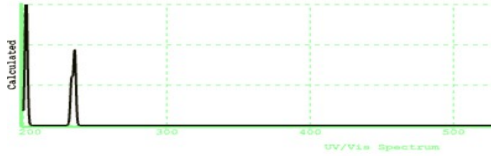
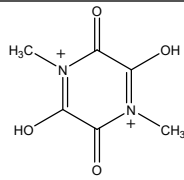
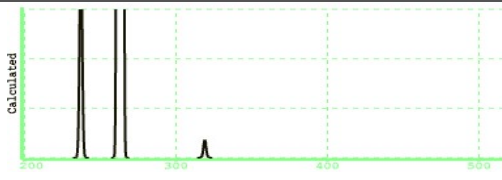
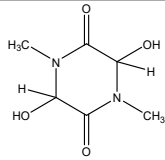
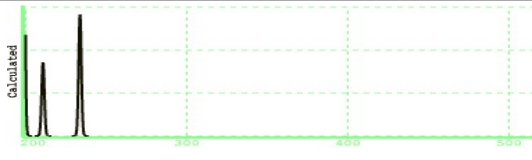
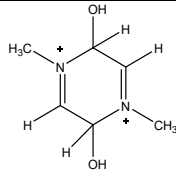
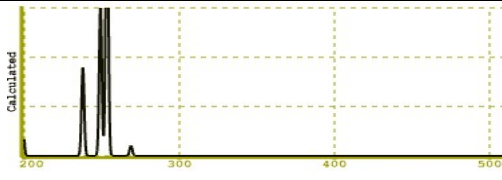
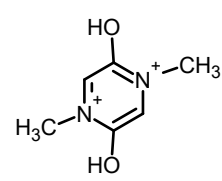
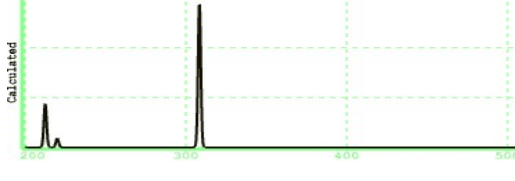
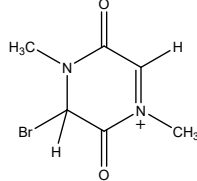
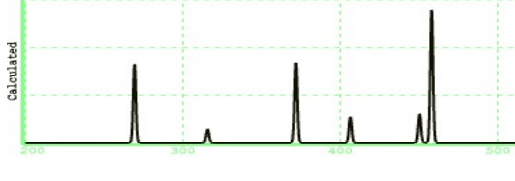
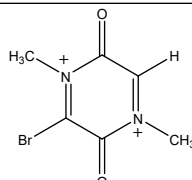
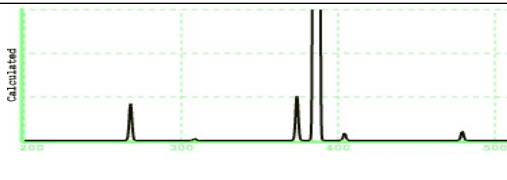
opoundt

### Quantum chemical calculations

DFT method using B3LYP functional and 6-31+G\* basis set as implemented in Spartan'18 was used for calculation of UV-vis spectra.

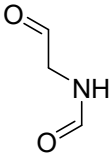
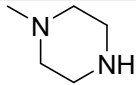
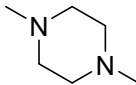
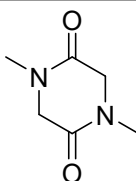
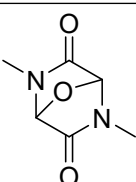
**Table S1**

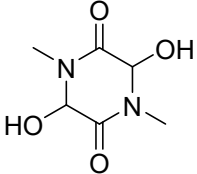
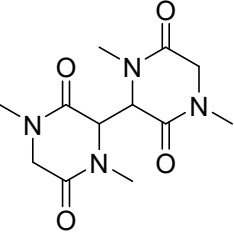
| Compound        | DFT Calculated Spectra |
|-----------------|------------------------|
| <p><b>1</b></p> |                        |
| <p><b>2</b></p> |                        |

|                                                                                     |                                                                                      |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------|
|    |    |
|    |    |
|    |    |
|    |    |
|   |   |
|  |  |
|  |  |
|  |  |
| $\lambda$                                                                           | 200                      300                      400 nm                             |

MS experiential data

Table S2

| Formula                                                                                                                                                                               | m/z                       |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|---------------------------|
|  <p>Chemical Formula: <math>C_3H_5NO_2</math><br/>m/z: 87.0320 (100.0%), 88.0354 (3.2%)</p>          | <p>87</p> <p>88</p>       |
|  <p>Chemical Formula: <math>C_5H_{12}N_2</math><br/>m/z: 100.1000 (100.0%), 101.1034 (5.4%)</p>      | <p>100.1</p>              |
|  <p>Chemical Formula: <math>C_6H_{14}N_2</math><br/>m/z: 114.1157 (100.0%), 115.1191 (6.5%)</p>      | <p>114.1</p> <p>115.1</p> |
|  <p>Chemical Formula: <math>C_6H_{10}N_2O_2</math><br/>m/z: 142.0742 (100.0%), 143.0776 (6.5%)</p> | <p>142</p> <p>143</p>     |
|  <p>Chemical Formula: <math>C_6H_8N_2O_3</math><br/>m/z: 156.0535 (100.0%), 157.0568 (6.5%)</p>    | <p>157</p> <p>157</p>     |

|                                                                                                                                                                                                                                 |                                           |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------|
|  <p>Chemical Formula: C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>O<sub>4</sub><br/>m/z: 174.0641 (100.0%), 175.0674 (6.5%)</p>                    | <p>174</p> <p>175</p>                     |
|  <p>Chemical Formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>4</sub><br/>m/z: 282.1328 (100.0%), 283.1362 (13.0%), 283.1298 (1.5%)</p> | <p>282.13</p> <p>283.14</p> <p>283.23</p> |

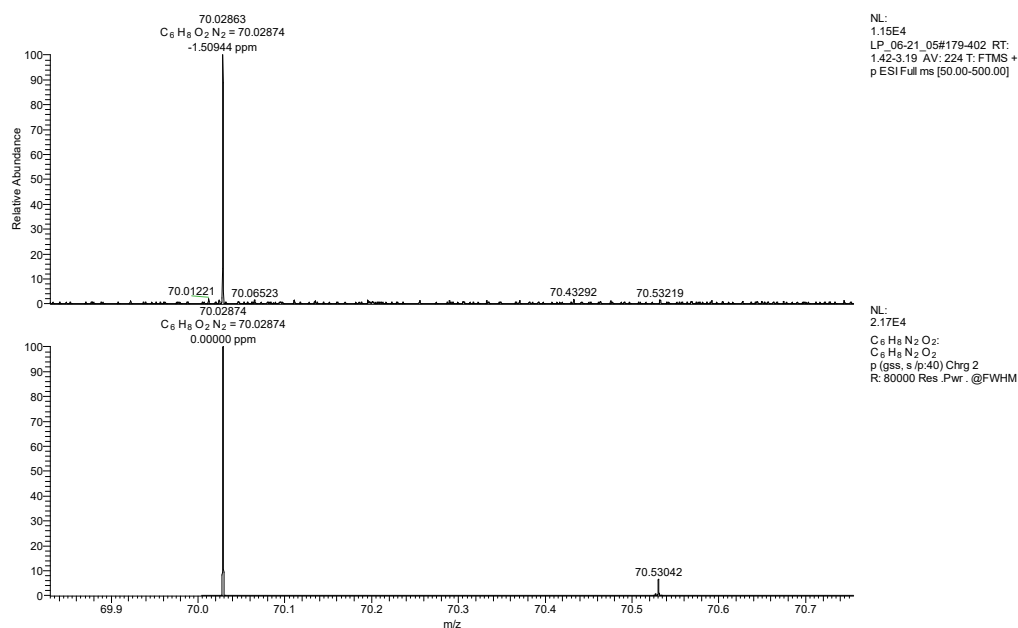


Figure S2 Section of the ESI+ mass spectrum of a solution of **1** treated with metallic mercury under argon (upper spectrum) and the simulated spectrum of the doubly charged compound **2** (lower spectrum). The sample was introduced via loop injection into acetonitrile flowing into the ion source.