Supporting Information

NMR spectra

In the $^1$H NMR spectrum of compound 3a (Figure 1), the signals of three meso-H (9.91; 9.91; for 9.88) and one proton signal of the azomethine group (10.40) are in low field.
Figure 1. $^1$H NMR spectrum of 3a and the low field fragment.
Figure 2. Fragment of NOESY spectrum of 3a.

Figure 3. Fragment of $^1$HNMR spectrum of isomers 3b + 3c.
Figure 4. $^1$HNMR spectrum 5.

Mass spectra

On the mass spectra of the four isomers of 3a-d two molecular ions are present, one corresponds to the Schiff base (M=768), and the other corresponds to cyclopentane derivative molecular ion (M=736) (Figure 5).
Figure 5. Fragment of the mass spectrum of isomers 3a-d.

Figure 6. Fragment of the mass spectrum of 4.
Electronic absorption spectra.

**Figure 7.** UV-Vis absorption spectra of 8 in acetone.

**Figure 8.** UV-Vis absorption spectra of 9 in acetone.
Figure 9. UV-Vis absorption spectra of 5 in acetone.

Figure 10. UV-Vis absorption spectra of 4 in acetone.

Photoluminescence spectra.
**Figure 11.** Photoluminescence spectra of 3a: measured (S1) and corrected (S1c).

**Figure 12.** Photoluminescence spectra of 3b+3c: measured (S1) and corrected (S1c).
**Figure 13.** Photoluminescence spectra of 3d: measured (S1) and corrected (S1c).

**Figure 14.** Photoluminescence spectra of 7: measured (S1) and corrected (S1c).
Figure 15. The phosphorescence spectrum of 8 in acetone at 77 K.

Figure 16. The phosphorescence spectrum of 9 in acetone at 77 K.
Figure 17. The phosphorescence spectrum of 5 in acetone at 77 K.

Figure 18. The phosphorescence spectrum of 4 in acetone at 77 K.
Figure 19. The time dependence of the phosphorescence of 3a.

Figure 20. The time dependence of the phosphorescence of 3b + 3c.
The calculation of the quantum yield of singlet oxygen generation.

Quantum yield of singlet oxygen generation by the studied compounds was determined by the relative method using chemical traps. The standard compound was TPP (mesotetraphenylporphin). According to literature data, the most probable value of the quantum yield of singlet oxygen generation by TPP in acetone was $0.65 \pm 0.05^{[1,2]}$. 1,3-Diphenylisobenzofuran (DPIBF) was used as a chemical trap. The interaction of this trap with singlet oxygen proceeds by chemical reaction is shown on the scheme below.\cite{3} The products of the reaction have no absorption bands in the visible spectrum. Therefore, the amount of singlet oxygen formed during the photoreaction can be measured by loss of optical density in the maximum absorption DPIBF.
Solutions of the investigated compounds and DPIBF in a fixed volume of solvent were prepared for the determination of quantum yields of singlet oxygen generation. Measurements were performed in square quartz fluorescence cuvettes with optical path length 1 cm. The solutions were irradiated for a certain time with the light from a xenon lamp fluorimeter Perkin Elmer MPF-44B passing through the monochromator. Light intensity was measured using a ThorLabs unit PM-100D with sensor head S120VC (Germany). Samples were irradiated with the wavelength of light, selected based on the position of the maximum wavelength of the green band of compound (550 nm). The spectral slit width of the monochromator of the fluorimeter corresponds to 5 nm. Not only the change of optical density at the maximum of absorption of DPIBF, but also at the wavelength of the exciting light was controlled at irradiation. During the irradiation the absorption band of the sensitizer do not fade, i.e. the optical density of sensitizer at the wavelength of the exciting light did not change. The optical density was determined using a two-beam spectrophotometer Hitachi U-3400. DPIBF concentration in the sample was selected so that its optical density in the maximum absorption was 0.80-1.10.

When calculating quantum yield by relative method the comparison of the loss of DPIBF optical density and the irradiation time in the experiments performed for the compound under investigation and standard compound. Three experiments were carried out with standard compound and four experiments were carried out with compound under investigation. The calculation was performed according to the following formula

$$\varphi_D = \varphi_{\Delta S} \cdot \frac{\Delta D_C \cdot t_{irr} \cdot I_S \cdot (1 - 10^{-D_C}) \cdot \lambda_S}{\Delta D_S \cdot t_{irrC} \cdot I_C \cdot (1 - 10^{-D_C}) \cdot \lambda_C}.$$

Where $\varphi_{\Delta S}$ is the quantum yield of generation of singlet oxygen standard compound; $\Delta D_C$ is the average loss of optical density of DPIBF in the experiments with the test compound, $\Delta D_S$ is the average loss of optical density DPIBF in experiments with the standard compound, $t_{irrC}$ is the duration of irradiation of the mixture DPIBF with compound under investigation in sec, $t_{irrS}$ is the duration of irradiation of the mixture CFIBF with standard compound in sec, $I_C$ and $I_S$ are intensities of the light flux from the xenon lamp in the experiments with the test connection and the standard compound in $\mu w$, $D_C$ and $D_S$ are optical densities of the compound under investigation and standard compound corresponding to the wavelengths of the exciting light $\lambda_C$ and $\lambda_S$ (in nm).
**Figure 23.** Absorption spectra of mixtures of 8 and DPIBF in acetone before and after irradiation at 550 nm in the presence of oxygen.

**Figure 24.** Absorption spectra of mixtures of 9 and DPIBF in acetone before and after irradiation at 550 nm in the presence of oxygen.
Figure 25. The kinetics of bleaching of DPIBF upon irradiation of the mixture with 9.

Figure 26. The UV-Vis absorption spectra of the mixture 5 and DPIBF in acetone before and after irradiation at 615 nm in the presence of oxygen.
Figure 27. The kinetics of bleaching of DPIBF upon irradiation of the mixture with 5.

Figure 28. The UV-Vis absorption spectra of the mixture 4 and DPIBF in acetone before and after irradiation at 613 nm in the presence of oxygen.
Table 1. Irradiation data of palladium complexes in the presence of DPIBF and oxygen in acetone.

<table>
<thead>
<tr>
<th>Compounds</th>
<th>λ, nm</th>
<th>I, µw</th>
<th>T_{irr}, s</th>
<th>ΔDc, ΔDst*</th>
<th>D_{c} or D_{st}*</th>
<th>φ</th>
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<tbody>
<tr>
<td>8 + DPIBF</td>
<td>550</td>
<td>94</td>
<td>120</td>
<td>0.136</td>
<td>0.115</td>
<td>1.00±0.07</td>
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<td>TPP + DPIBF</td>
<td>512</td>
<td>105</td>
<td>600</td>
<td>0.112</td>
<td>0.026</td>
<td>0.65±0.05</td>
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<tr>
<td>9 + DPIBF</td>
<td>545</td>
<td>97</td>
<td>120</td>
<td>0.14</td>
<td>0.114</td>
<td>1.00±0.05</td>
</tr>
<tr>
<td>TPP + DPIBF</td>
<td>512</td>
<td>105</td>
<td>600</td>
<td>0.112</td>
<td>0.026</td>
<td>0.65±0.05</td>
</tr>
<tr>
<td>5 + DPIBF</td>
<td>615</td>
<td>107</td>
<td>120</td>
<td>0.176</td>
<td>0.116</td>
<td>1.00±0.05</td>
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<tr>
<td>TPP + DPIBF</td>
<td>512</td>
<td>105</td>
<td>600</td>
<td>0.112</td>
<td>0.026</td>
<td>0.65±0.05</td>
</tr>
<tr>
<td>4 + DPIBF</td>
<td>613</td>
<td>98</td>
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<tr>
<td>TPP + DPIBF</td>
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<td>600</td>
<td>0.113</td>
<td>0.026</td>
<td>0.65±0.05</td>
</tr>
</tbody>
</table>

* Averaged values across multiple experiments.

References: