Electronic Supplementary Information

New Thiocyanate-Free Ruthenium(II) Sensitizers with different Pyrid-2-yl tetrazolate Ligands for Dye-Sensitized Solar Cells

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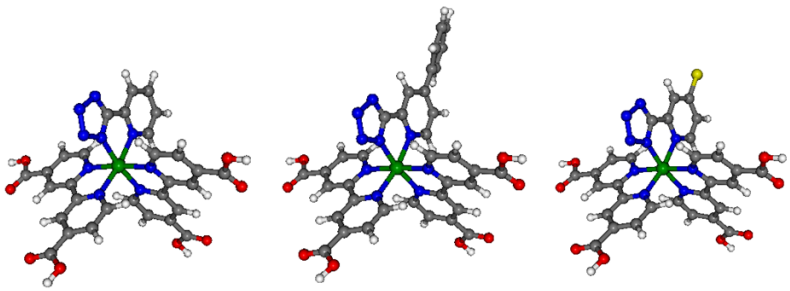

1 **2** **3**

Figure S1. Optimized geometries of investigated dyes.

Table S1. Experimental and calculated absorption maxima wavelengths (in nm) and excitation energy (in eV). Also the excitation energy differences between experimental and theoretical values were reported.

	Experimental	**Calculated**	
	λ_{max} (nm/eV)	**λ_{max} (nm/eV)**	**Δ E (eV)**
1	496/2.49 440/2.81 37/3.31	475/2.60 445/2.78 380/3.25	0.11 0.03 0.05
2	497/2.49 444/2.79 385/3.21	477/2.59 449/2.76 380/3.25	0.10 0.03 0.04
3	492/2.51	470/2.63	0.12

	441/2.81 378/3.27	443/2.80 379/3.26	0.01 0.01

Table S2. Excitation energies, oscillator strengths and excited state wave-function composition of investigated dyes.

Compound	**N_state**	**E (eV)**	**WL (nm)**	**f**	**Composition(%)**	
1	5	2.60	476	0.25	H-2 →L H-1 →L+1	47 34
	6	2.78	445	0.04	H-2 →L+1 H-1 →L+1	33 23
	8	3.13	396	0.13	H →L+4	71
2	5	2.58	480	0.25	H-2 →L H-1 →L+1	64 27
	6	2.76	449	0.06	H-2 →L	57
	8	3.12	398	0.15	H →L+4	71
3	5	2.63	472	0.25	H-2 →L H-1 →L+1	53 33
	6	2.80	443	0.05	H-2 →L+1 H-1 →L+1	38 20
	8	3.16	393	0.14	H →L+4	72

Table S3. Calculated molecular orbitals energies (eV) in DMSO solvent of investigated dyes. The energies were calculated at B3LYP/ DGDZVP level.

	1	**2**	**3**
L+3	-2.67	-2.67	-2.68
L+2	-2.71	-2.71	-2.72
L+1	-3.26	-3.26	-3.27

L	-3.35	-3.35	-3.36
H	-6.42	-6.42	-6.47
H-1	-6.58	-6.53	-6.62
H-2	-6.66	-6.62	-6.69
H-3	-7.35	-7.25	-7.49
H-L Gap	3.07	3.07	3.11
$S_0 \rightarrow S_1$	2.25	2.25	2.28

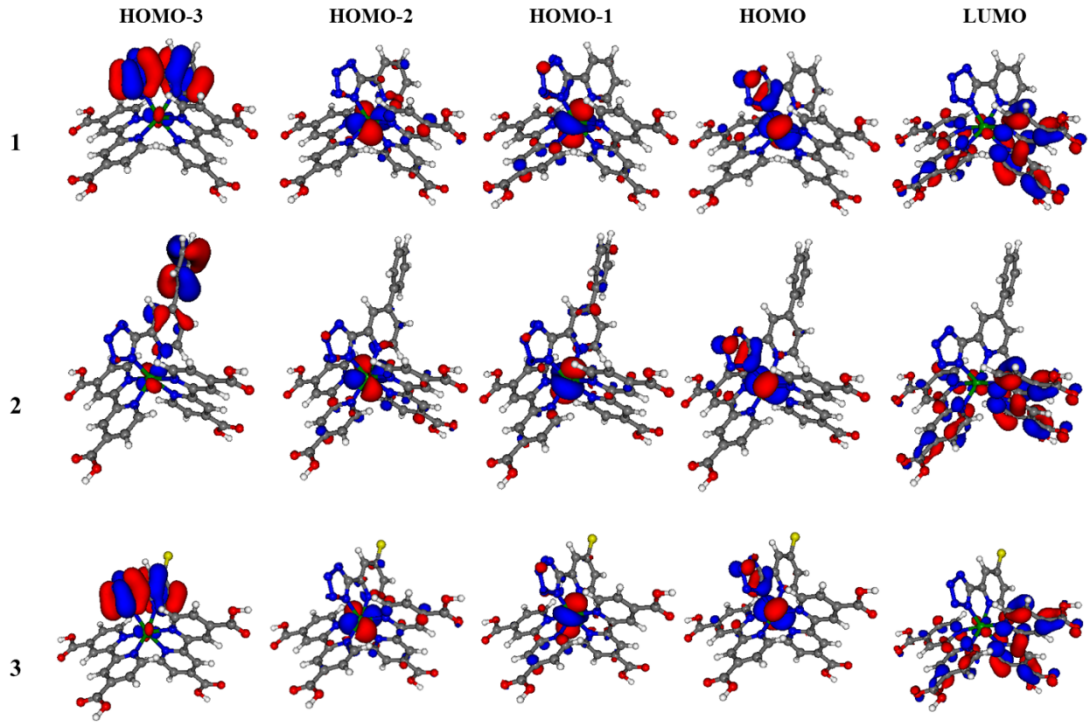

Figure S2. Isodensity plots of relevant molecular orbitals of investigated dyes.

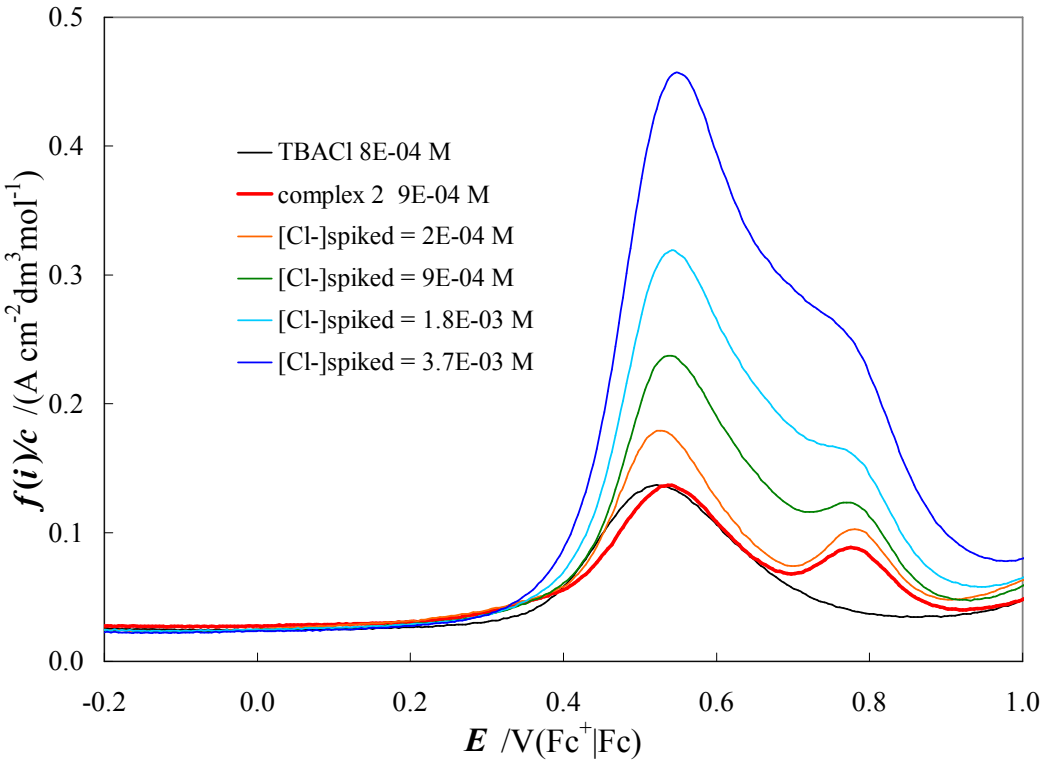

Figure S3. Synopsis of differential pulse voltammograms on GC electrode (0.071 cm^2) employed for the clarification of the nature of the two anodic peaks observed for complexes **1-3**. The figure represents DPV patterns for complex **2** alone ($9 \cdot 10^{-4}$ M, red thick line) and after subsequent additions of TBACl as source of Cl^- anions. For sake of comparison the pattern of a $8 \cdot 10^{-4}$ M TBACl solution (black thin line) in the same condition is reported. Conditions: DMF + $TBAPF_6$ 0.1 M; potential scan rate 0.05 V s^{-1}.

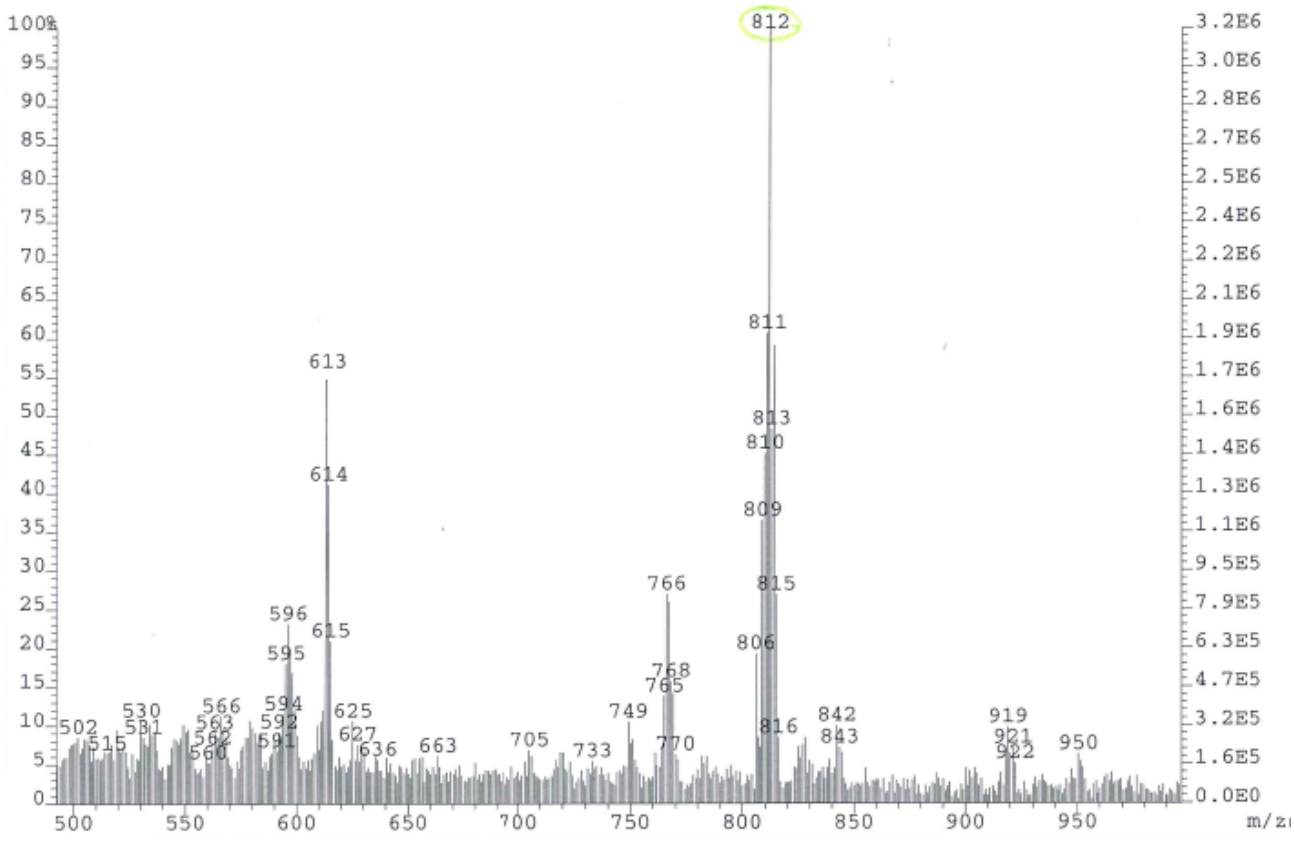

Figure S4 FAB$^+$ spectrum of complex **2** after treatment with *tert*-butylpyridine.

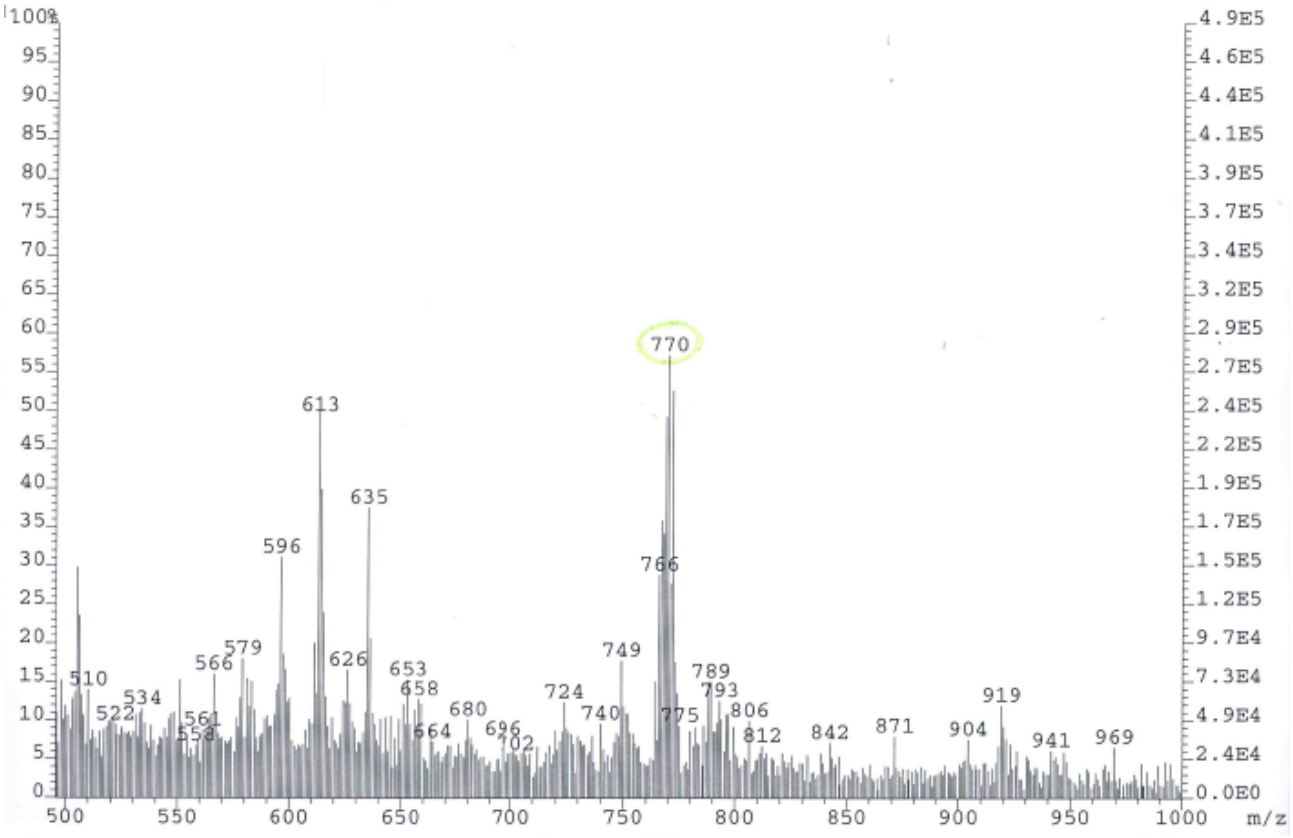

Figure S5 FAB$^+$ spectrum of complex **3** after treatment with *tert*-butylpyridine.