Supplementary Material

Uranyl N_2O_2-Schiff Base Complex as Co-catalyst in Ethanol Electro-oxidation: Synthesis, Crystallographic, Spectroscopic, Electrochemical, and DFT Characterization, and Catalytic Investigation

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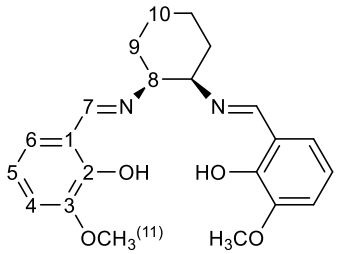
List of Tables

List of Figures

Table S1. ^{1}H (400 MHz) and ^{13}C (100 MHz) data of H_2L and $[UO_2(L)H_2O]$ in DMSO-d_6 (25 °C) with tetramethylsilane (TMS), as internal standard (chemical shifts in ppm and *J* in Hz).



	H_2L		$[UO_2(L)H_2O]$	
	δ ^{1}H (multiplicity, *J* Hz)	δ ^{13}C	δ ^{1}H (multiplicity, *J* Hz)	δ ^{13}C
1	-	118.35	-	123.7
2	-	151.69	-	159.7
3	-	148.03	-	150.9
4	7.00 (*m*)	117.68	7.22 (*dd*, 7.8, 1.5)	116.5
5	6.79 (*t*, 7.88)	114.55	6.61 (*t*, 7.8)	115.4
6	7.00 (*m*)	123.21	7.25 (*dd*, 7.8, 1.5)	126.4
7	8.55 (*s*)	165.29	9.40 (*s*)	167.8
8	3.68 (*d*, 5.68)	67.75	4.63-4.55 (*m*)	70.6
9	1.80 (*m*), 1.55 (*m*)	30.42	2.40-2.20 (*m*) 1.88-1.72 (*m*) 1.68-1.58 (*m*)	27.5
10		21.91		21.4
11	3.74 (*s*)	55.62	3.97 (*s*)	56.1
OH	13.51 (*s*)	-	-	-

s = singlet, *d* = doublet, *dd* = doublet of doublets, *t* = triplet, *m* = multiplet.

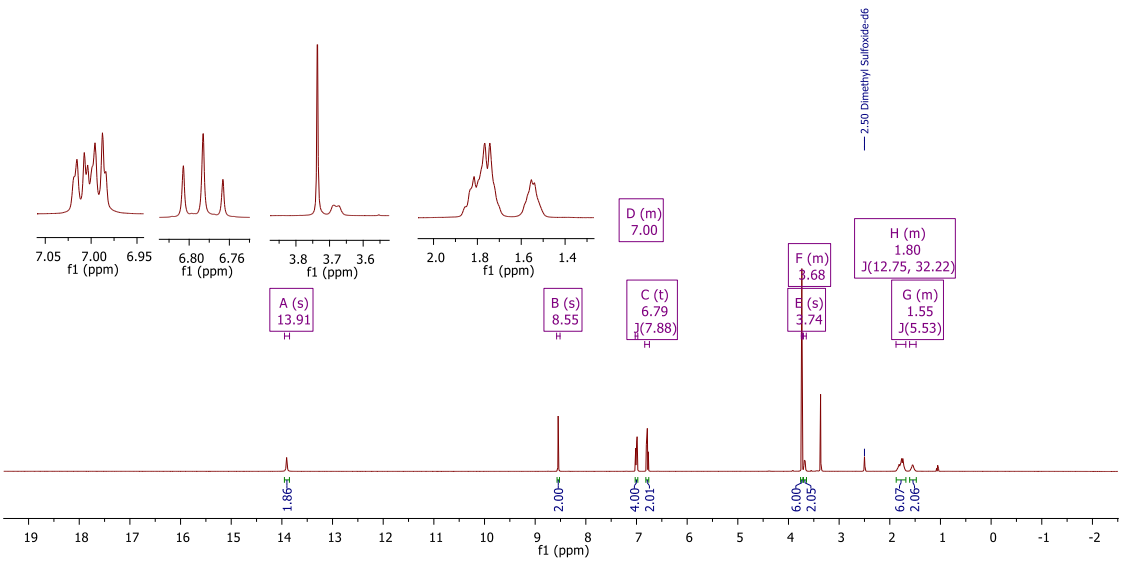


Figure S1. ^{1}H NMR spectrum (400 MHz, DMSO-d_6) for 3-OMe-*c*-salcn.

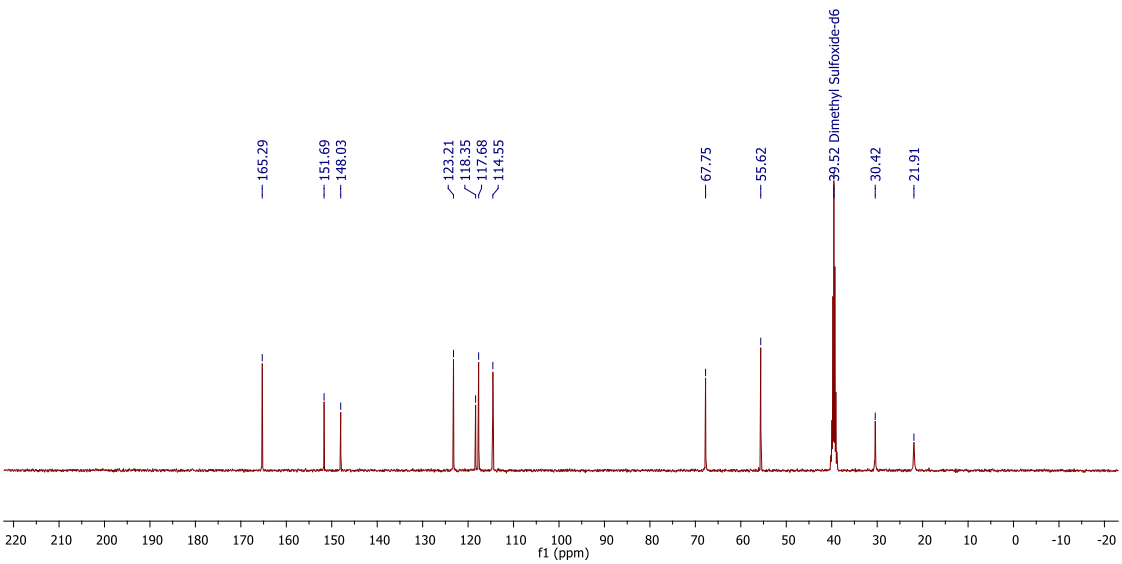


Figure S2. ^{13}C NMR spectrum (100 MHz, DMSO-d_6) for 3-OMe-*c*-salcn.

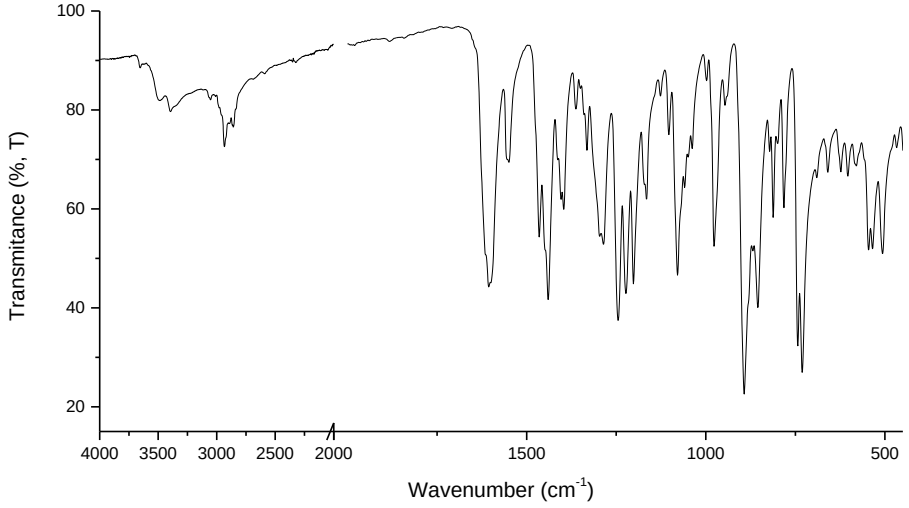


Figure S3. Infrared spectra (4000-450 cm^{-1}, KBr) for [UO_2(3OMe-*c*-salcn)H_2O].

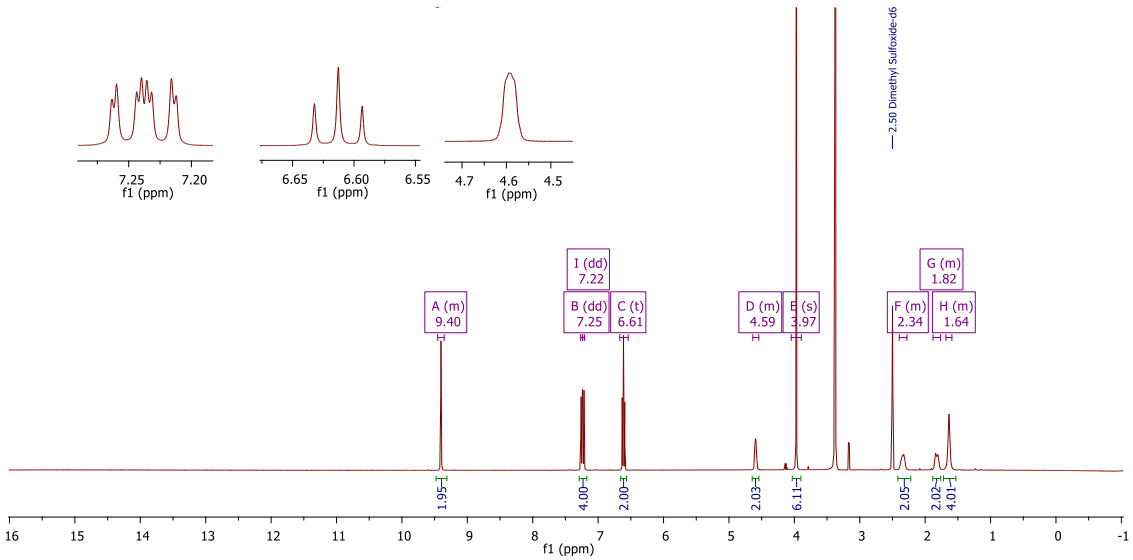


Figure S4. ^1H NMR spectrum (400 MHz, DMSO-d_6) for [UO_2(3OMe-*c*-salcn)H_2O].

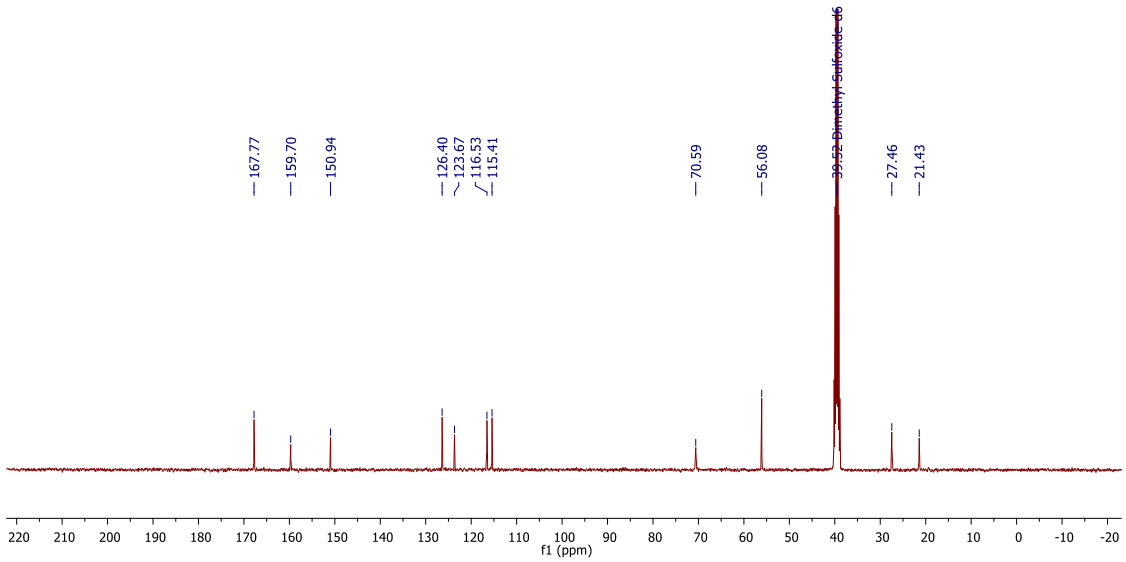


Figure S5. ^{13}C NMR spectrum (400 MHz, DMSO-d_6) for [UO_2(3OMe-*c*-salcn)H_2O].

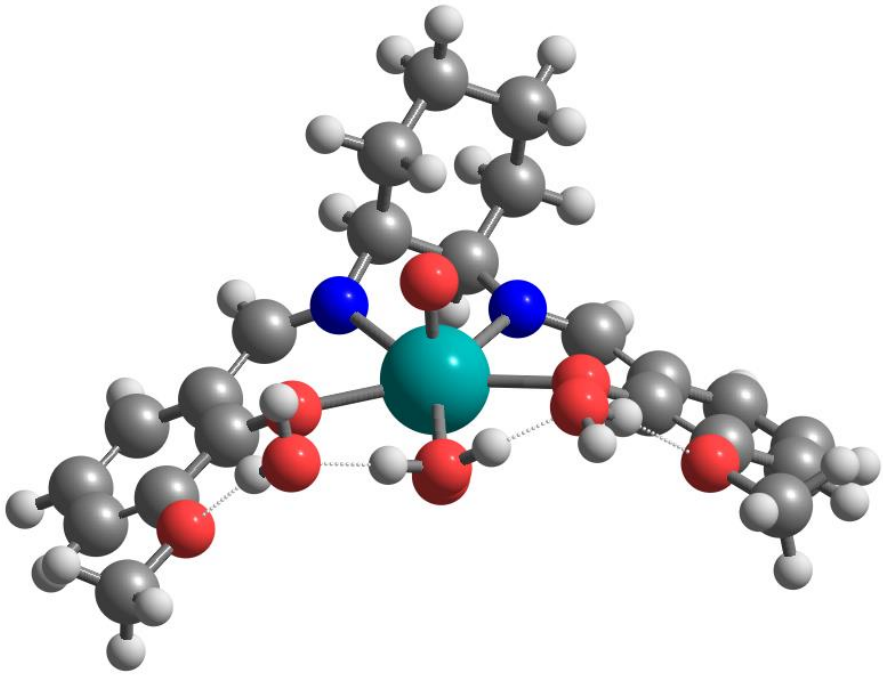


Figure S6. Optimized geometry for *cis*-[UO_2(3-OMe-*c*-salcn)(H_2O)] at DKH-PBE/Def2-TZVPP-D3BJ//SARC-TZVPP level of theory.

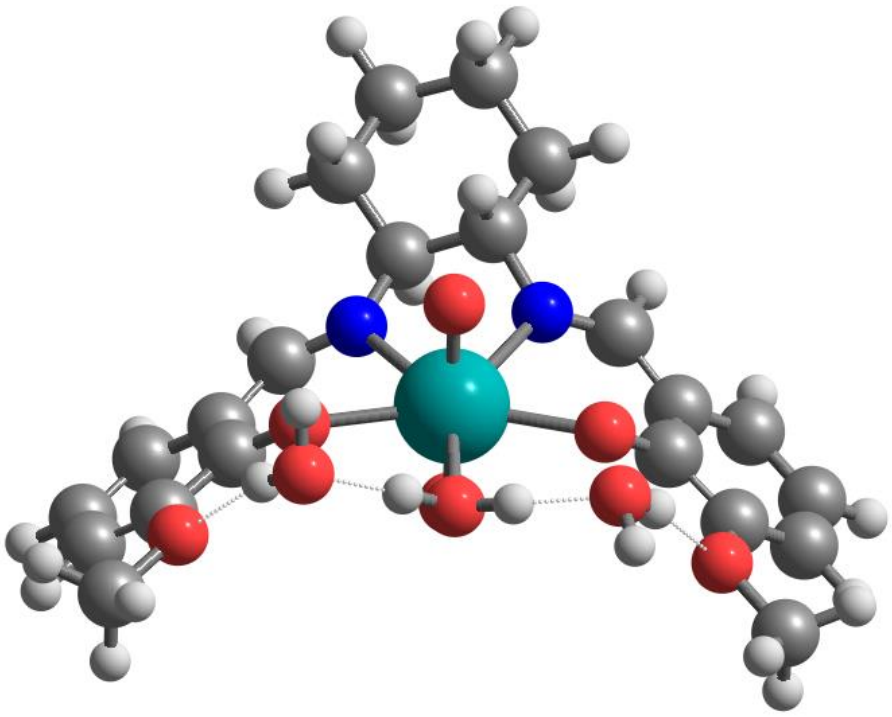


Figure S7. Optimized geometry for *trans*-[UO_2(3-OMe-*c*-salcn)(H_2O)] at DKH-PBE/Def2-TZVPP-D3BJ//SARC-TZVPP level of theory.

Table S2. Experimental (190-800 nm, Acetonitrile, 25°C) and theoretical (ZORA-PBE/Def2-TZVPP-3BJ//SARC-TZVPP – SMD-Acetonitrile) UV-Vis attribution (λ in nm and ε in $L^{\bullet}mol^{-1\bullet}cm^{-1}$).

Comp	Experimental				Theoretical	Assignment
	Observed		G. A			
	$\lambda_{máx}$	$\varepsilon_{máx}$	$\lambda_{máx}$	$\varepsilon_{máx}$	$\lambda_{máx}$	
[UO_2(L)H_2O]					1003	LMCT ($p\pi \rightarrow f\pi$)
					835	LMCT
					616	LMCT ($p\pi \rightarrow f\pi$)
			482	33		-
	344	7311	401	1900	411	LMCT ($p\pi \rightarrow f\pi$) $\pi \rightarrow \pi^*$

		347	4400		LMCT
268	21500	282	10300		LMCT
		268	8800		π→ π*(N=C)
236	61000	239	31600		π→ π*(C=C)
		229	35900		π→ π*(C=C)

G.A – Gaussian analysis

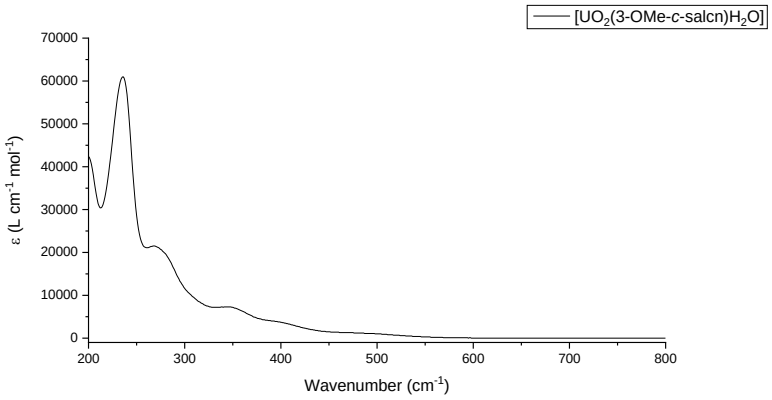


Figure S8.[UO_2(3-OMe-*c*-salcn)H_2O] UV-Vis electronic spectra (200-800 nm, acetonitrile, 25°C).

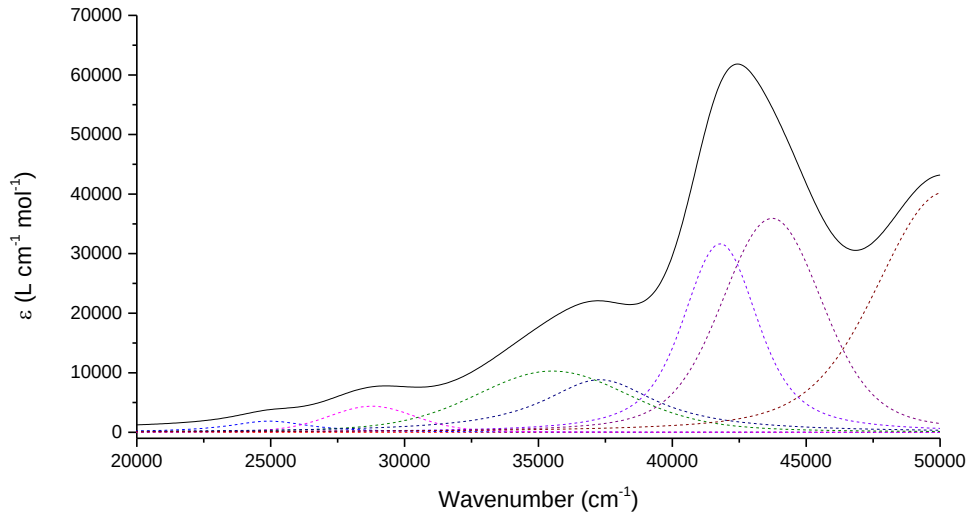


Figure S9. Gaussian analysis of [UO_2(3-OMe-*c*-salcn)H_2O] for electronic spectrum in the 50000-20000 cm^{-1} (200-500 nm, Acetonitrile, 25°C) region.

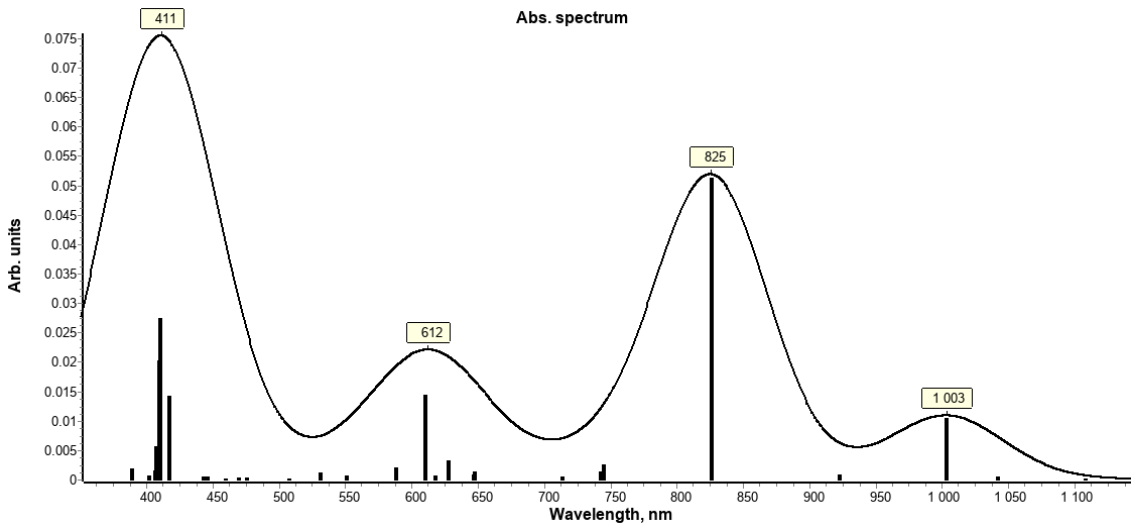
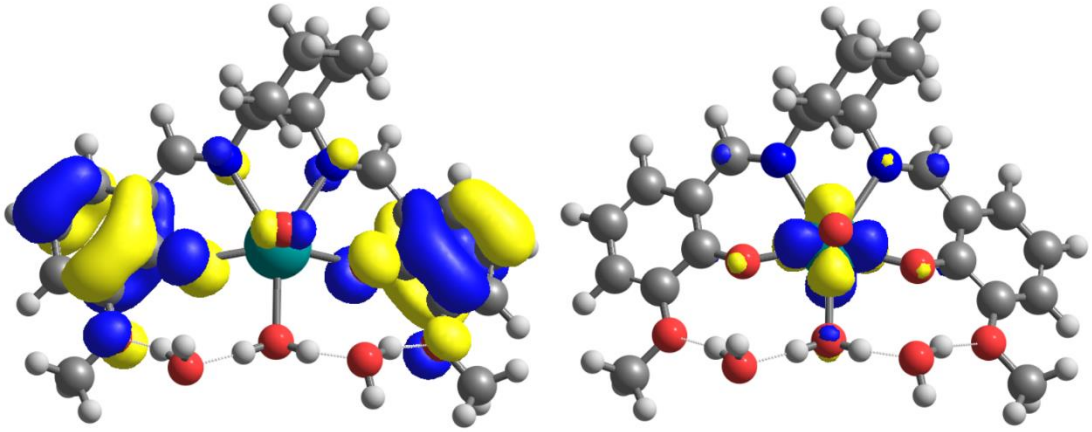
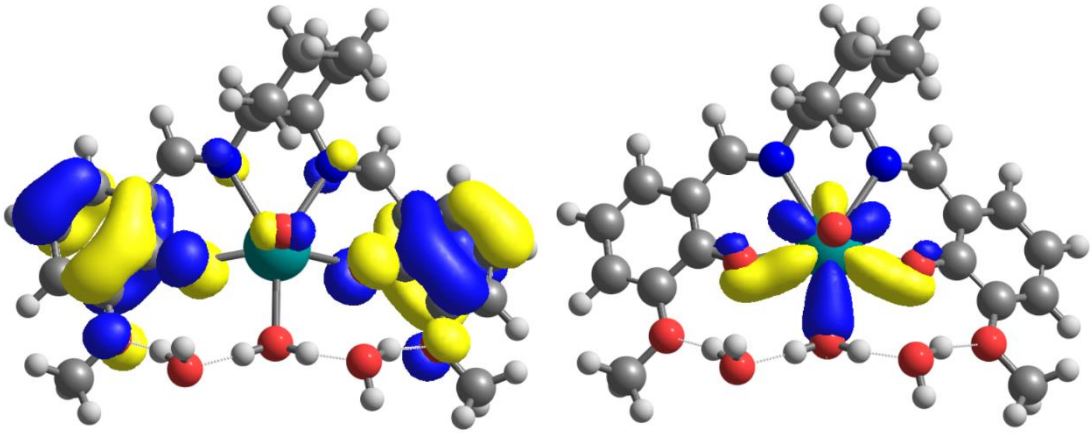


Figure S10. UV-VIS spectrum for [UO_2(3-OMe-*c*-salcn)H_2O] calculated at ZORA-PBE/Def2-TZVPP-3BJ//SARC-TZVPP (SMD-acetonitrile) level of theory.



(HOMO) (LUMO+1)

Figure S11. Molecular orbitals involved at calculated light absorption process of [UO_2(3-OMe-*c*-salcn)H_2O] at 1003 nm.



(HOMO) (LUMO+2)

Figure S12. Molecular orbitals involved at calculated light absorption process of [UO_2(3-OMe-*c*-salcn)H_2O] at 835 nm.

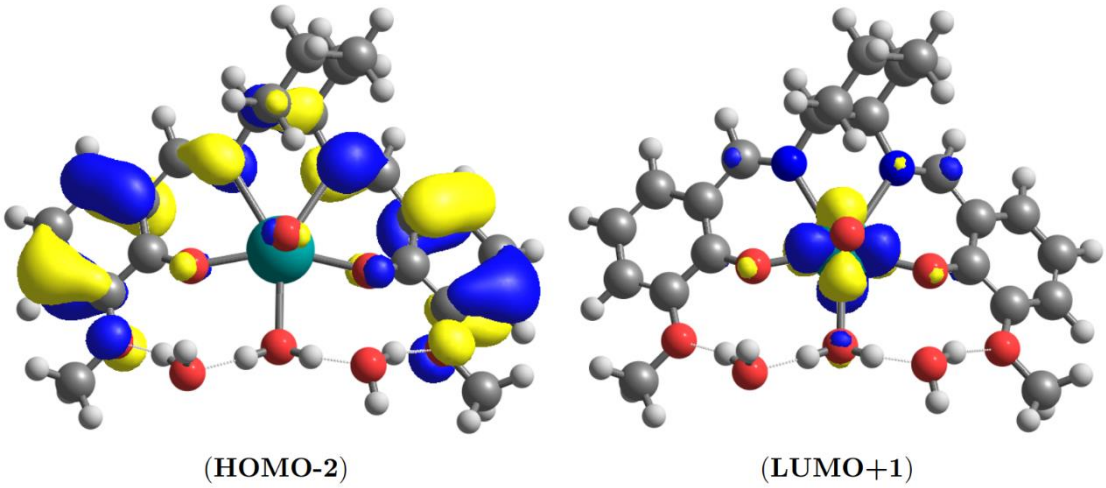
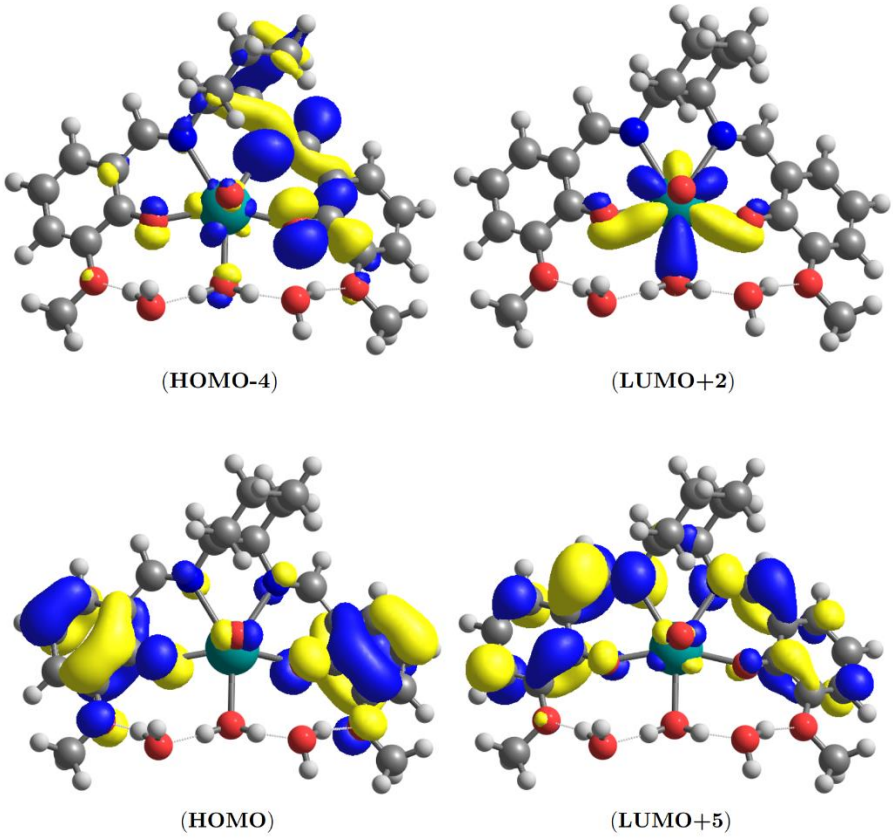


Figure S13. Molecular orbitals involved at calculated light absorption process of [UO_2(3-OMe-*c*-salcn)H_2O] at 612 nm.



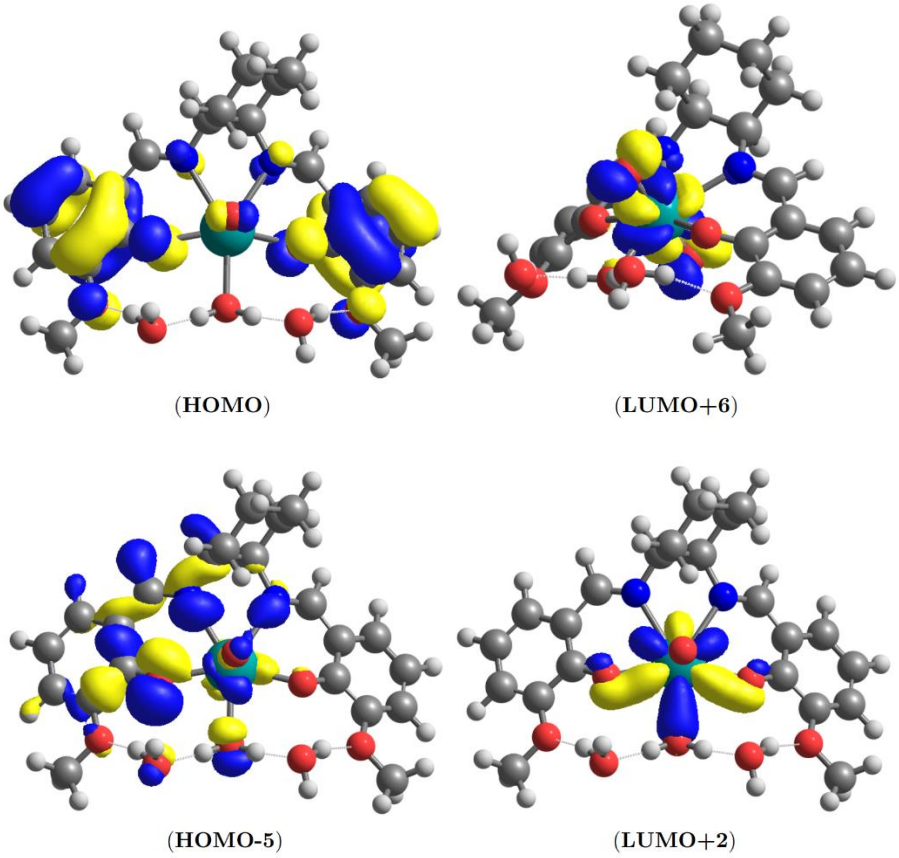


Figure S14. Molecular orbitals involved at calculated light absorption processes of [UO_2(3-OMe-*c*-salcn)H_2O] around 411 nm.