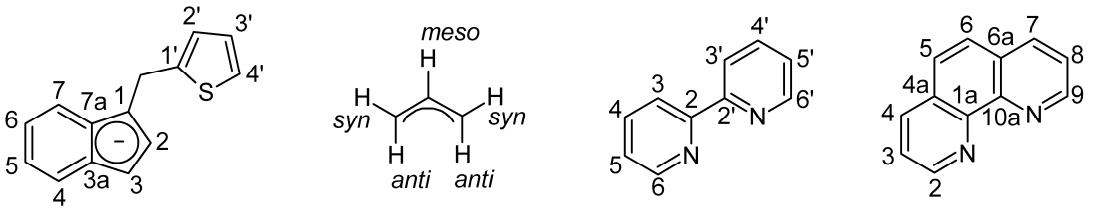
Numbering scheme of the used ligands



Scheme S1

Table S1 Crystallographic data for complexes 2 and 4

	2	**4**
empiric formula	$C_{19}H_{16}MoO_2S$	$C_{26}H_{19}MoN_2O_2SBF_4$
crystal system	monoclinic	monoclinic
space group	$P2_1/n$	$P2_1/n$
a[Å]	9.7184(7)	10.435(6)
b[Å]	8.1432(6)	13.950(8)
c[Å]	20.7926(14)	17.033(9)
α[°]	90	90
β[°]	100.207(2)	98.418(16)
γ[°]	90	90
Z	4	4
μ[mm^{-1}]	0.945	0.678
D_x[Mgm^{-3}]	1.658	1.642
cryst size [mm]	0.365×0.234×0.191	0.333×0.274×0.244
υ range [°]	2.5–27.5	1.9–27.5
T_{min}, T_{max}	0.78, 0.84	0.81, 0.85
no. reflections measured	33951	22750
no. of unique reflns, R_{int}[a]	3734, 0.012	5656, 0.020
no. of observed reflns [I>2σ(I)]	3643	4804
no. of parameters	229	362
S[b] all data	1.116	1.036
final R[b] indices [I>2σ(I)]	0.020	0.020
wR2[b] indices (all data)	0.022	0.087
Δρ, max., min. [eÅ^{-3}]	0.497, -0.763	0.669, -0.965
no. CCDC	1853493	1853492

[a] $R_{int} = \Sigma \left| F_o^2 - F_{o,mean}^2 \right| / \Sigma F_o^2$, [b] $S = [\Sigma(w(F_o^2 - F_c^2)^2)/(N_{diffrs} - N_{params})]^{½}$. [b] $R(F) = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$, $wR(F^2) = [\Sigma(w(F_o^2 - F_c^2)^2)/(\Sigma w(F_o^2)^2)]^{½}$

Stability of complex 6

For the evaluation of the stability of the most active compound **6**, the complex was firstly dissolved in methanol and then diluted with water to obtain 1:1 (MeOH:H_2O) solution. After that, the mass spectroscopy and UV/VIS were recorded. Subsequently, the solution was stirred at room temperature for 24 hours and the spectra were recorded again.

Electronic absorption spectra were run on a Black-Comet C-SR-100 concave grating spectrometer (region 200 - 1080 nm, optical pathway 1 and 0.1 cm). Mass spectrometry was performed with a quadrupole mass spectrometer (LCMS 2010, Shimadzu, Japan). The sample was injected into the mass spectrometer with infusion mode at a constant flow rate of 10 µl/min. Electrospray ionization-mass spectrometry (ESI-MS) was used for the identification of analyzed samples. The experimental data are summarized in Table S2.

Table S2 UV/VIS data of complex **6** measured in 1:1 mixture MeOH:H_2O.

Time (h)	λ_{max1} [nm]	λ_{max2} (ε)
0	287	527
24	287	525

The UV/VIS spectrum of the compound **6** shows two main absorption bands at 287 and 527 nm with the extinction coefficients of 53966 and 8235 l mol^{-1} cm^{-1} respectively. After the stirring of the solution for 24 h the UV/VIS spectrum does show any signs of decomposition. The stability was also proved by MS spectra were the base peak with the m/z value of 697 corresponds to $[M]^+$ fragment.