Supplemental Data

Influence of supporting ligand microenvironment on the aqueous stability and visible light induced CO release reactivity of zinc flavonolato species

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Figure S1. ¹H NMR spectrum of [(6-Ph₂TPA)Zn(3-Hfl)]ClO₄ (**1**) in CD₃CN at 25 °C. * denotes residual Et₂O; ** denotes residual CH₂Cl₂ in the sample.

Figure S2. ¹H NMR spectrum of [(TPA)Zn(3-Hfl)]ClO₄ (**3**) in CD₃CN at 25 °C.

Figure S3. ¹H NMR spectrum of [(TPA)Zn(3-Hfl)]ClO₄ (**3**) at various temperatures in CD₂Cl₂.

Figure S4. MALDI mass spectrum of [(TPA)Zn(3-Hfl)]ClO₄ (**3**).

Figure S5. ¹H NMR spectrum of [(bnpapa)Zn(3-Hfl)]ClO₄ (**4**) in CD₃CN at 25 °C. * denotes residual Et₂O; ** denotes residual CH₂Cl₂ in the sample.

Figure S6. MALDI mass spectrum of [(bnpapa)Zn(3-Hfl)]ClO₄ (**4**).

Figure S7. ¹H NMR spectrum of [(TPA)Zn(*O*-bs)]ClO₄ (**5**) in CD₃CN at 25 °C.

Figure S8. MALDI mass spectrum of [(TPA)Zn(*O*-bs)]ClO₄ (**5**).

Figure S9. MALDI mass spectrum of [(TPA)Zn(*O*-bs-¹⁸O₂)]ClO₄ (**5-¹⁸O₂**).

Figure S10. ¹H NMR spectrum of [(bnpapa)Zn(*O*-bs)]ClO₄ (**6**) in CD₃CN at 25 °C.

Figure S11. MALDI mass spectrum of [(bnpapa)Zn(*O*-bs)]ClO₄ (**6**).

Figure S12. MALDI mass spectrum of [(bnpapa)Zn(*O*-bs-¹⁸O₂)]ClO₄ (**6-¹⁸O₂**).

Figure S1. ^1H NMR spectrum of $[(6\text{-Ph}_2\text{TPA})\text{Zn}(3\text{-Hfl})]\text{ClO}_4$ (**1**) in CD_3CN at 25°C . * denotes residual Et_2O ; ** denotes residual CH_2Cl_2 in the sample.

Figure S2. ^1H NMR spectrum of $[(\text{TPA})\text{Zn}(\text{3-Hfl})]\text{ClO}_4$ (3) in CD_3CN at $25\text{ }^\circ\text{C}$. Note: The grouping of resonances at $\sim 8.5\text{--}9.0$ ppm integrates to 6 H's. This indicates that one of the H's listed for the other aromatic group is located here. However, we are unable to assign which hydrogen this may be.

Figure S3. ^1H NMR spectra of $[(\text{TPA})\text{Zn}(\text{3-Hfl})]\text{ClO}_4$ (**3**) at various temperatures in CD_2Cl_2 .

#492

Measured Mass

591.1385

Element	Low Limit	High Limit
C	28	38
H	15	35
N	0	5
O	0	5
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C35 H29 N O4 Zn	591.1383	0.2	0.4	22
C36 H25 N5 Zn	591.1396	-1.1	-1.8	27
C33 H27 N4 O3 Zn	591.1369	1.6	2.7	22.5
C38 H27 N2 O Zn	591.1409	-2.4	-4.1	26.5

Figure S4. MALDI mass spectrum of $[(\text{TPA})\text{Zn}(\text{3-Hfl})]\text{ClO}_4$ (**3**).

Figure S5. ^1H NMR spectrum of $[(\text{bnpapa})\text{Zn}(\text{3-Hfl})]\text{ClO}_4$ (**4**) in CD_3CN at $25\text{ }^\circ\text{C}$. * denotes residual Et_2O ; ** denotes residual CH_2Cl_2 in the sample.

#491

Measured Mass

761.312

Element	Low Limit	High Limit
C	38	48
H	40	60
N	4	8
O	0	5
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C38 H49 N8 O5 Zn	761.3112	0.8	1.1	18.5
C43 H49 N6 O3 Zn	761.3152	-3.2	-4.2	22.5

Figure S6. MALDI mass spectrum of [(bnpapa)Zn(3-Hfl)]ClO₄ (**4**).

Figure S7. ^1H NMR spectrum of $[(\text{TPA})\text{Zn}(\text{O-bs})]\text{ClO}_4$ (5) in CD_3CN at 25°C .

#493

Measured Mass

579.1376

Element	Low Limit	High Limit
C	27	37
H	20	40
N	0	5
O	0	5
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C34 H29 N O4 Zn	579.1383	-0.7	-1.1	21
C32 H27 N4 O3 Zn	579.1369	0.7	1.2	21.5
C35 H25 N5 Zn	579.1396	-2.0	-3.4	26

Figure S8. MALDI mass spectrum of [(TPA)Zn(*O*-bs)]ClO₄ (**5**).

#500

Measured Mass

599.1407

<u>Element</u>	<u>Low Limit</u>	<u>High Limit</u>
C	27	37
H	20	40
N	2	6
O	0	2
18O	0	2
Zn	0	1

<u>Formula</u>	<u>Calculated Mass</u>	<u>mDaError</u>	<u>ppmError</u>	<u>RDB</u>
C32 H27 N4 O2 18O2 Zn	599.1403	0.4	0.6	21.5
C34 H25 N6 18O Zn	599.1418	-1.1	-1.9	25.5
C35 H27 N4 O2 Zn	599.1420	-1.3	-2.2	24.5
C36 H27 N3 O 18O Zn	599.1432	-2.5	-4.1	25

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Figure S9. MALDI mass spectrum of $[(\text{TPA})\text{Zn}(\text{O-bs-}^{18}\text{O}_2)]\text{ClO}_4$ ($5\text{-}^{18}\text{O}_2$).

Figure S10. ^1H NMR spectrum of $[(\text{bnpapa})\text{Zn}(\text{O-bs})]\text{ClO}_4$ (**6**) in CD_3CN at $25\text{ }^\circ\text{C}$.

#499

Measured Mass			765.3124
Element	Low Limit	High Limit	
C	37	47	
H	40	50	
N	4	8	
O	0	5	
Zn	0	1	

Formula	Calculated Mass	mDaError	ppmError	RDB
C45 H47 N7 O Zn	765.3128	-0.4	-0.5	26
C47 H49 N4 O2 Zn	765.3141	-1.7	-2.3	25.5
C42 H49 N6 O4 Zn	765.3101	2.3	3.0	21.5

Figure S11. MALDI mass spectrum of $[(\text{bnpapa})\text{Zn}(\text{O-bs})]\text{ClO}_4$ (**6**).

#502

Measured Mass

769.3196

Element	Low Limit	High Limit
C	37	47
H	40	60
N	5	7
O	0	3
18O	0	3
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C43 H49 N5 O 18O3 Zn	769.3198	-0.2	-0.2	22
C45 H49 N6 O2 Zn	769.3203	-0.7	-0.9	24.5
C42 H49 N6 O2 18O2 Zn	769.3186	1.0	1.3	21.5
C46 H49 N5 O 18O Zn	769.3215	-1.9	-2.4	25
C41 H49 N7 O3 18O Zn	769.3174	2.2	2.8	21
C38 H49 N7 O3 18O3 Zn	769.3158	3.8	5.0	18

Figure S12. MALDI mass spectrum of [(bnpapa)Zn(*O*-bs-¹⁸O₂)]ClO₄ (**6**-¹⁸O₂).