Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

Solution or solid – it doesn't matter: Visible light-induced CO release reactivity of zinc flavonolato complexes

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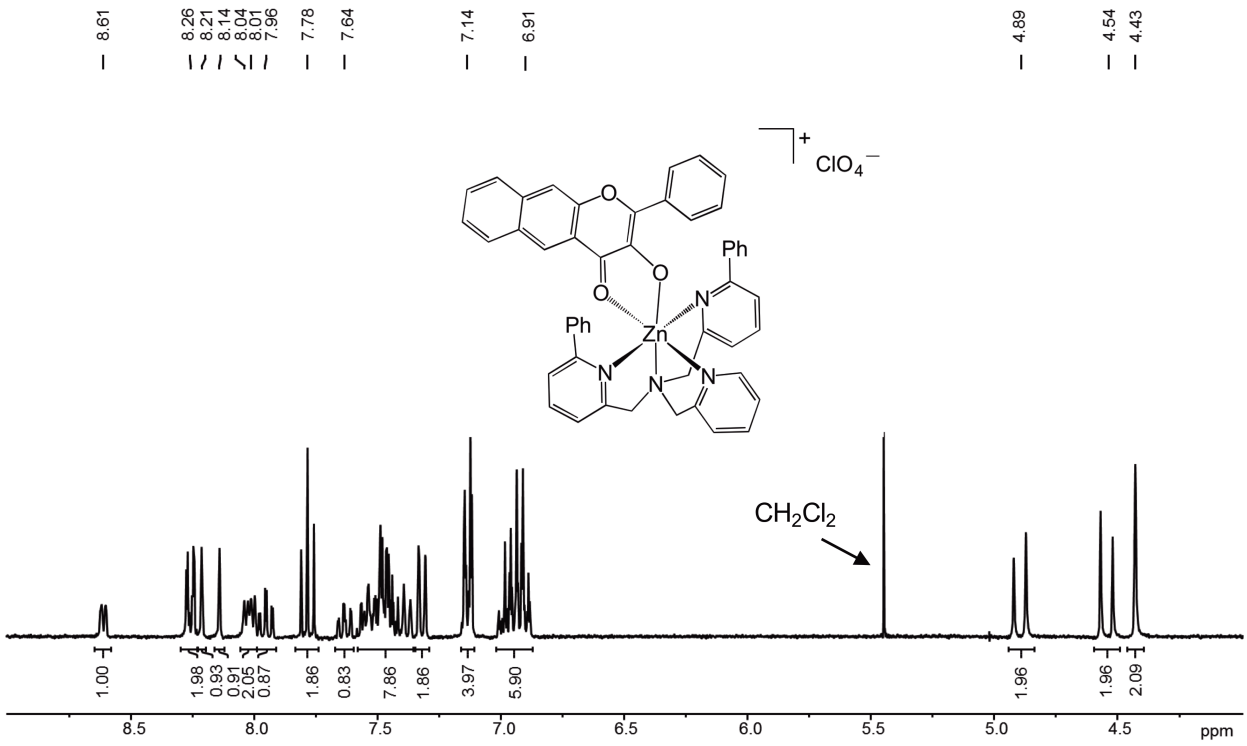


Figure S1. ^{1}H NMR of **5** in CD_3CN.

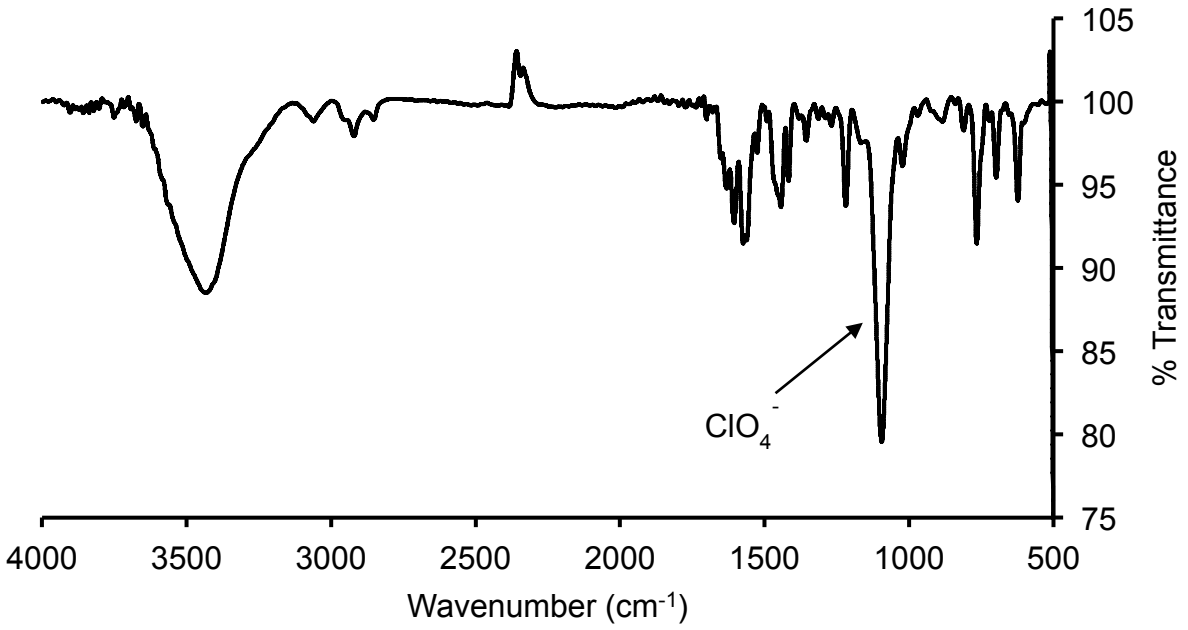


Figure S2. FT-IR spectrum of **5** in KBr.

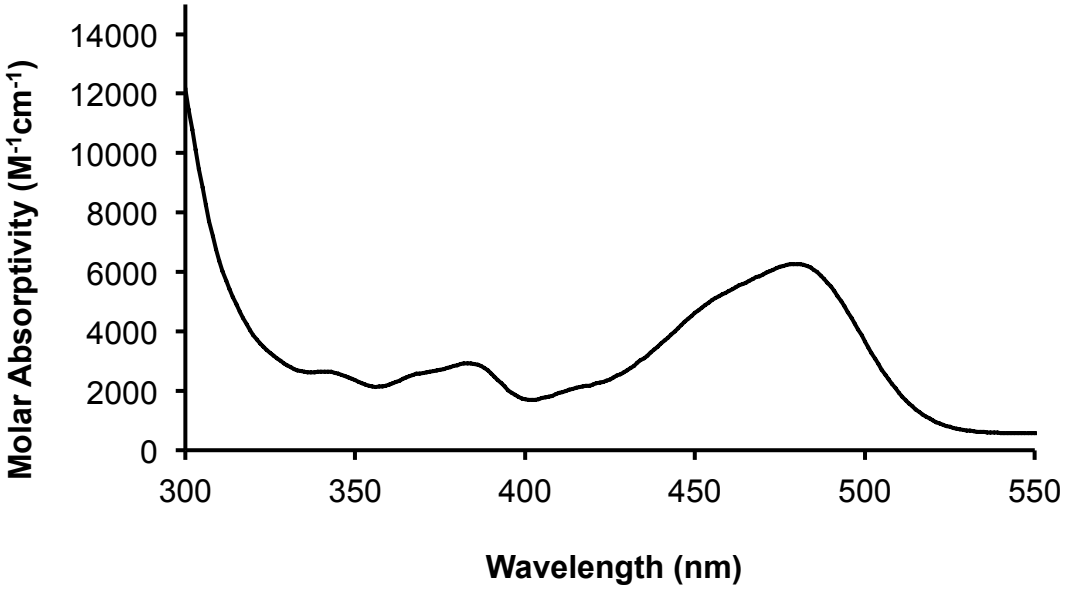


Figure S3. Absorption spectrum of **5** in acetonitrile.

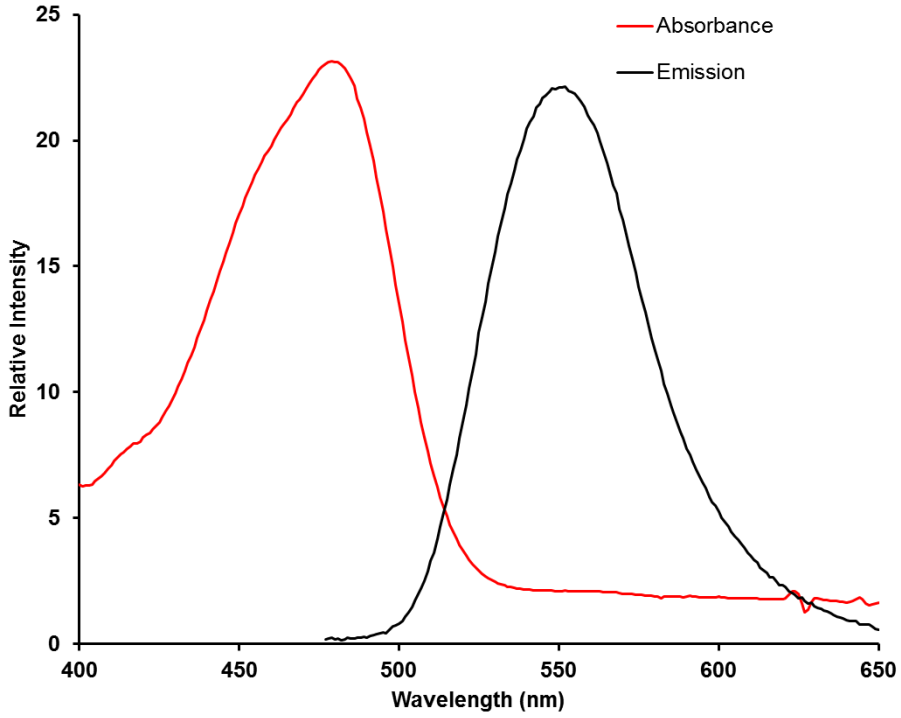
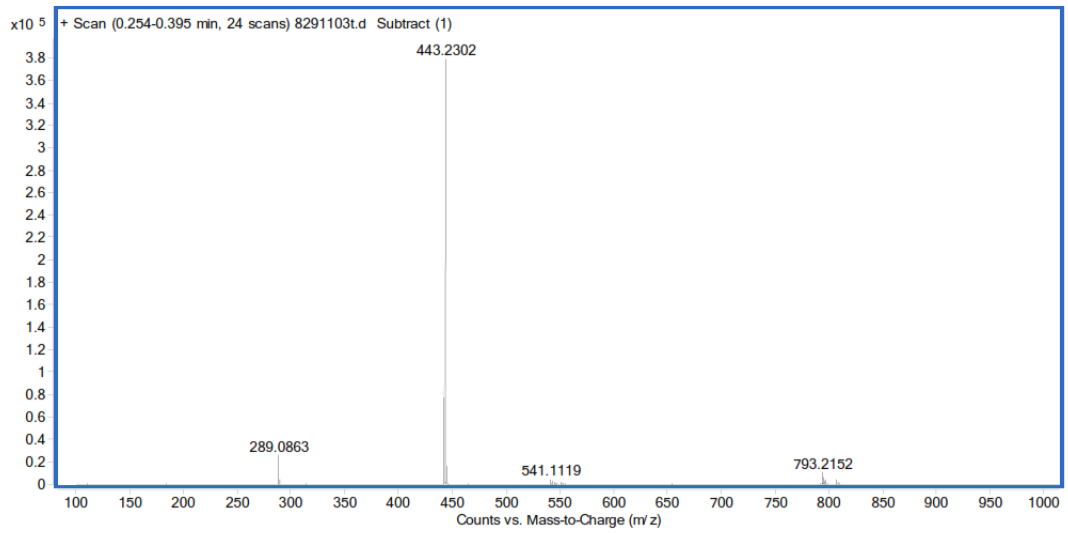
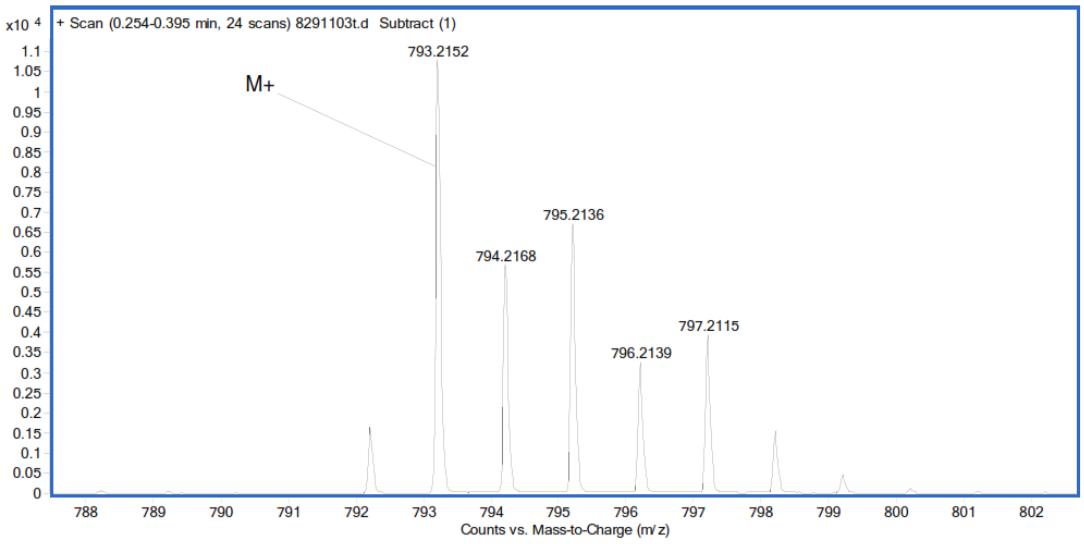


Figure S4. Overlay of the lowest energy absorption feature of **5** with the emission spectrum of **5** in acetonitrile.





Measured Mass	793.2152	
Element	**Low Limit**	**High Limit**
C	44	54
H	30	50
N	2	6
O	0	5
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C49 H37 N4 O3 Zn	793.2152	0.0	0.0	33.5
C52 H35 N5 Zn	793.2178	-2.6	-3.3	38

Figure S5. ESI/APCI MS of **5**.

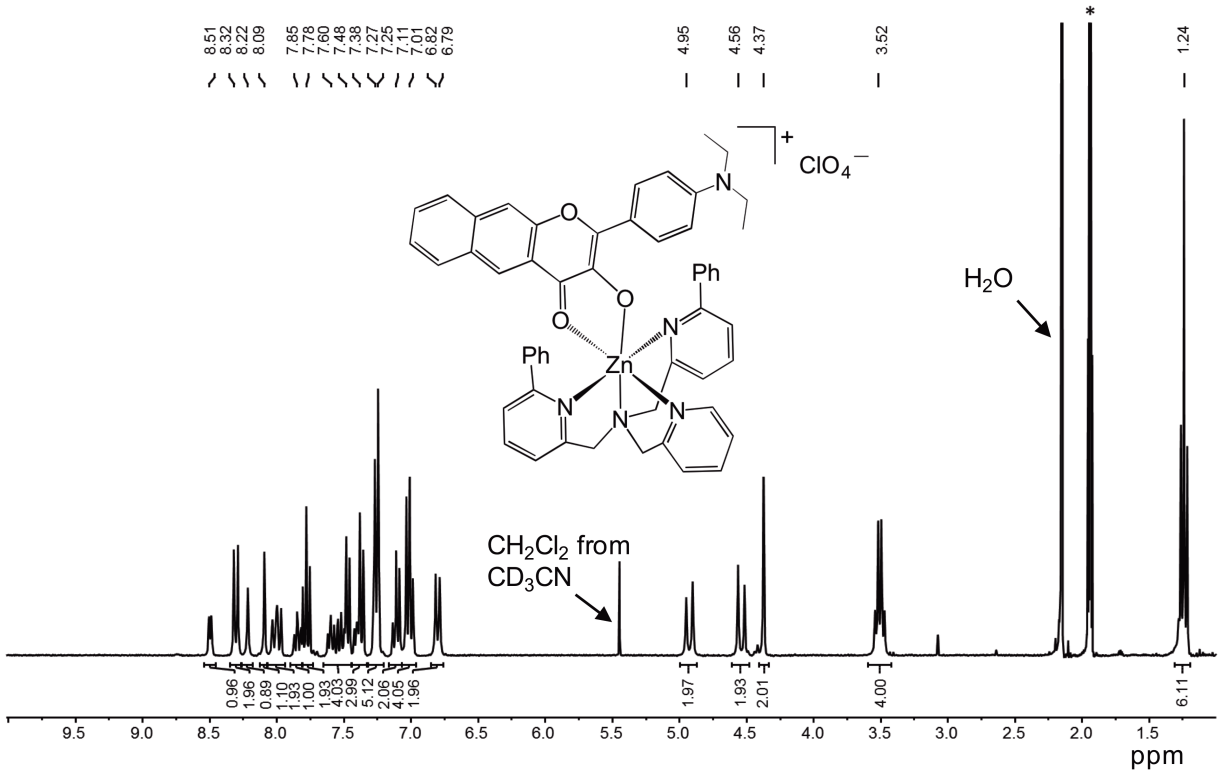


Figure S6. ^{1} H NMR spectrum of **6** in CD_3CN. (*denotes residual solvent)

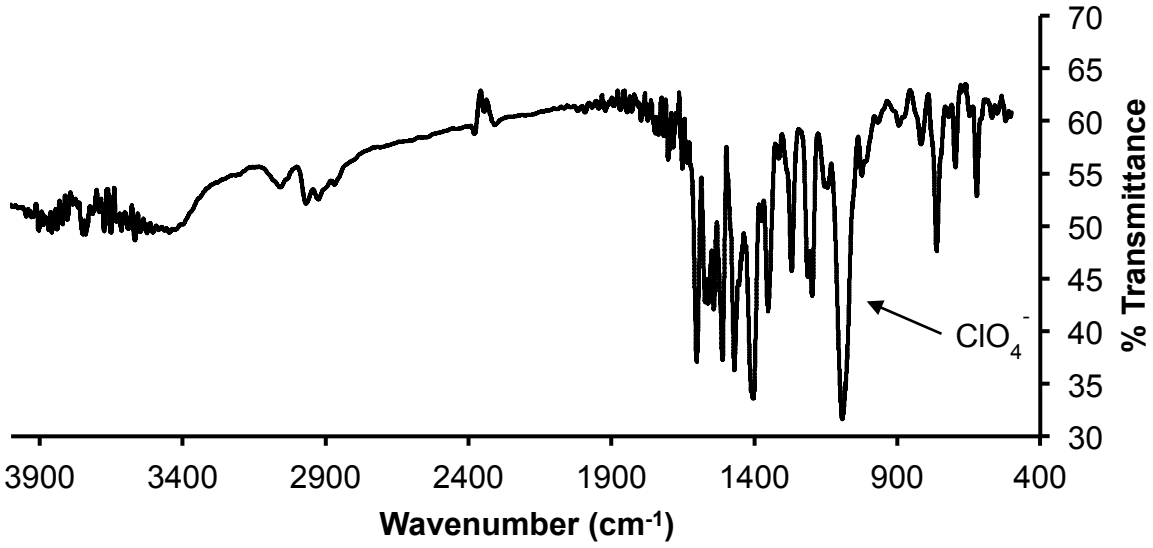


Figure S7. FT-IR of **6** in KBr.

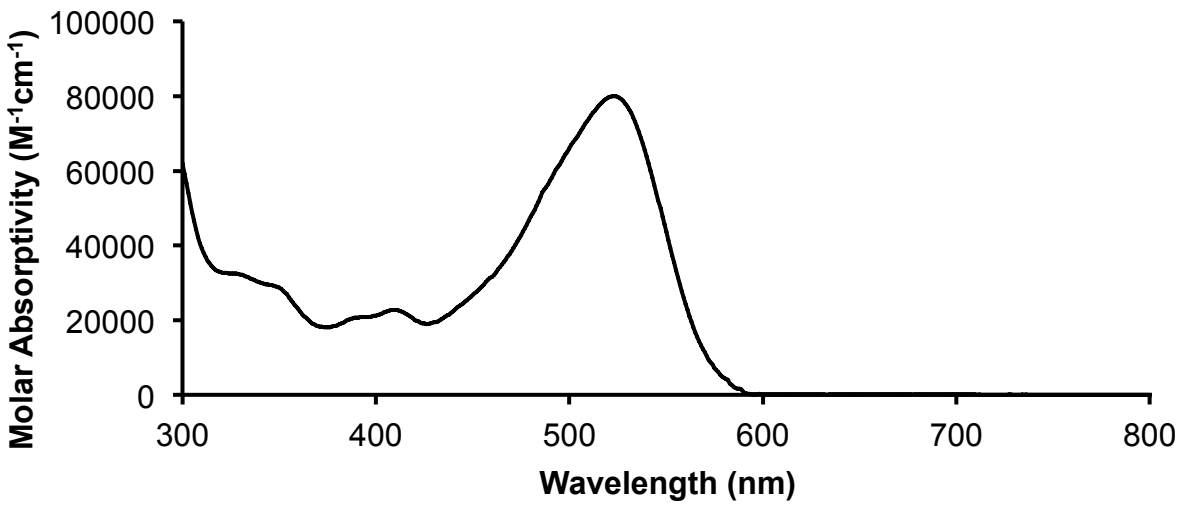


Figure S8. Absorption spectrum of **6** in acetonitrile.

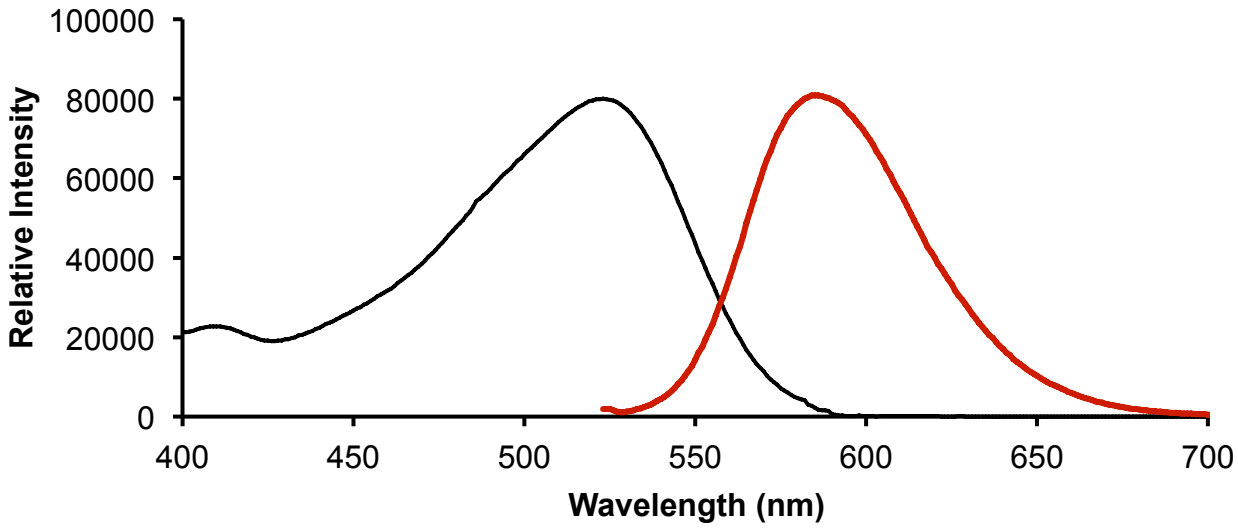
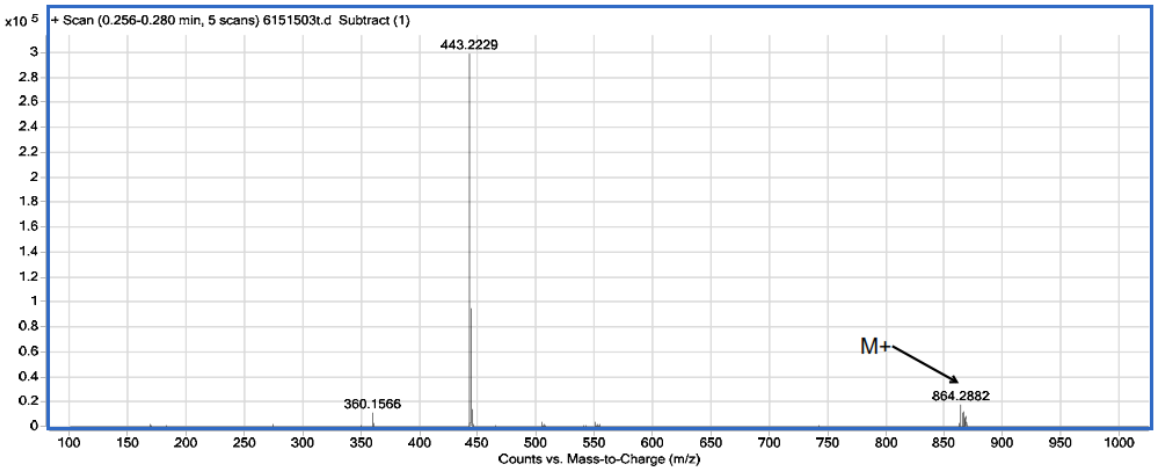
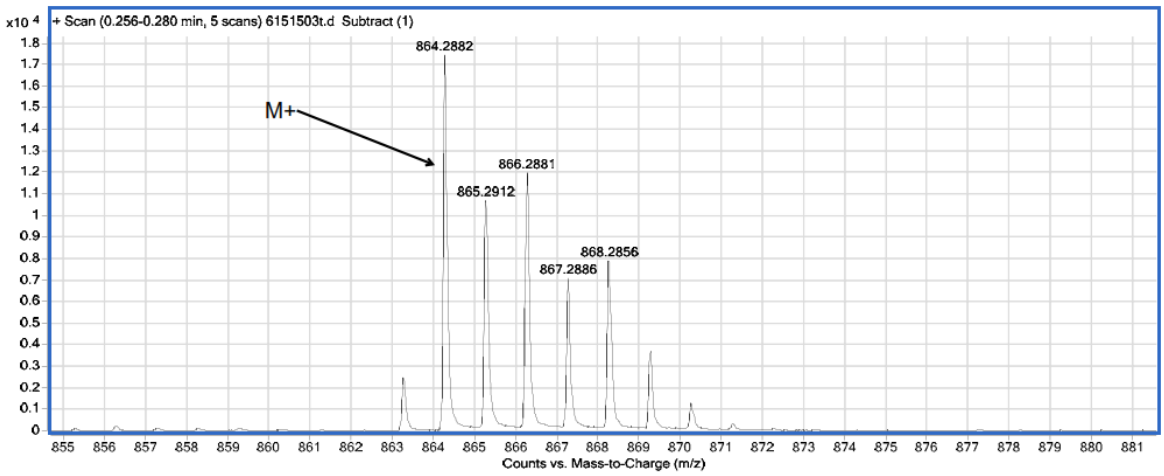


Figure S9. Overlay of the lowest energy absorption feature of **6** (black) with the emission spectrum (red) in acetonitrile.





Measured Mass	864.2882	
Element	**Low Limit**	**High Limit**
C	48	58
H	35	55
N	3	7
O	2	6
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C53 H46 N5 O3 Zn	864.2887	-0.5	-0.5	33.5
C50 H48 N4 O6 Zn	864.2860	2.2	2.6	29
C48 H46 N7 O5 Zn	864.2846	3.6	4.1	29.5
C58 H36 N6 O3	864.2843	3.9	4.5	44

Figure S10. ESI/APCI MS of **6**.

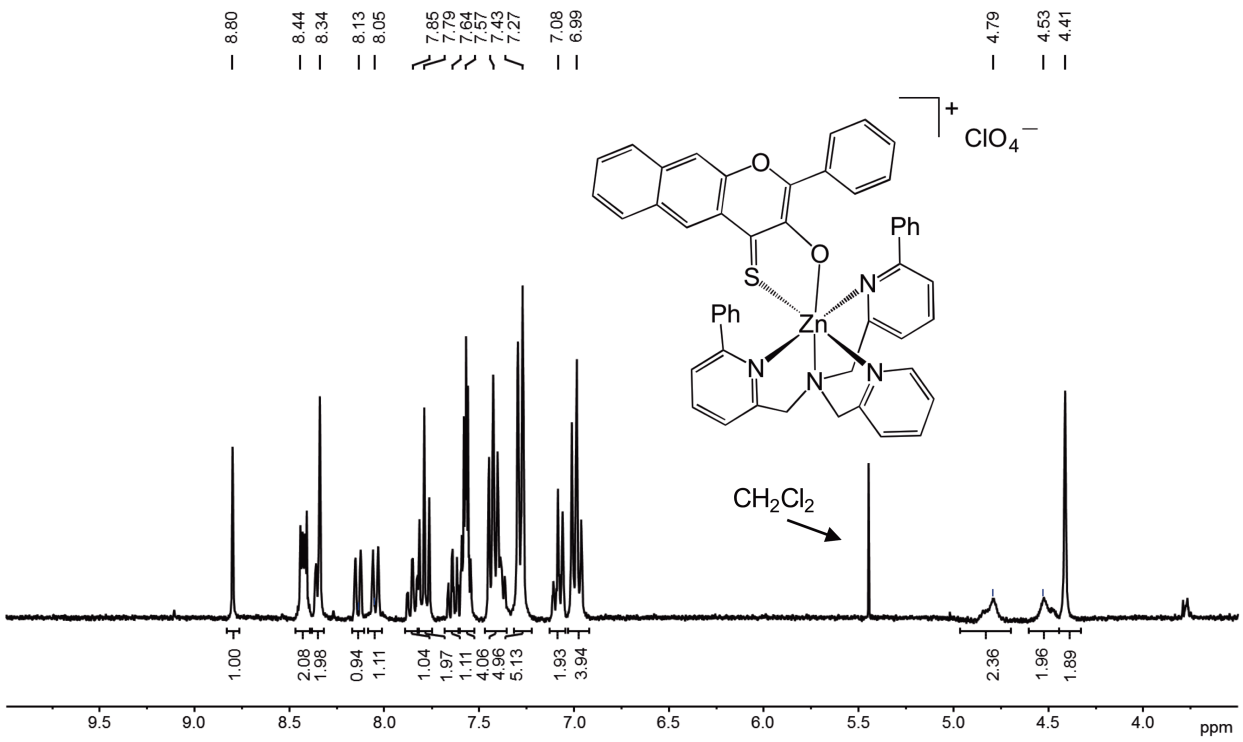


Figure S11. ^{1}H NMR of **7** in CD_3CN.

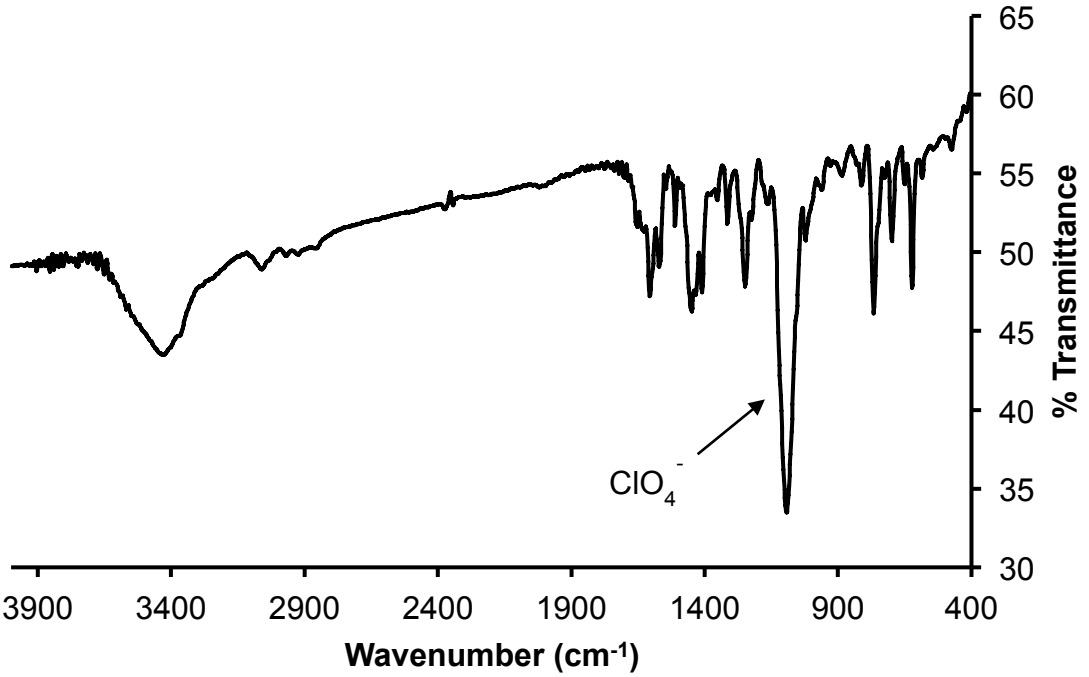


Figure S12. FT-IR of **7** in KBr.

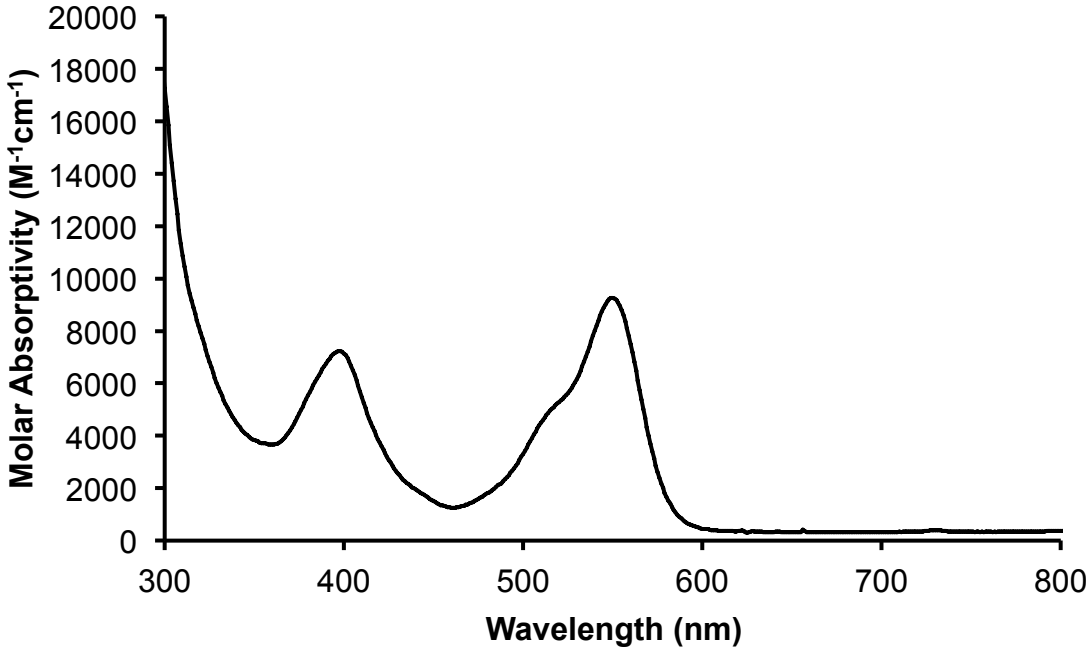


Figure S13. Absorption spectrum of **7** in acetonitrile.

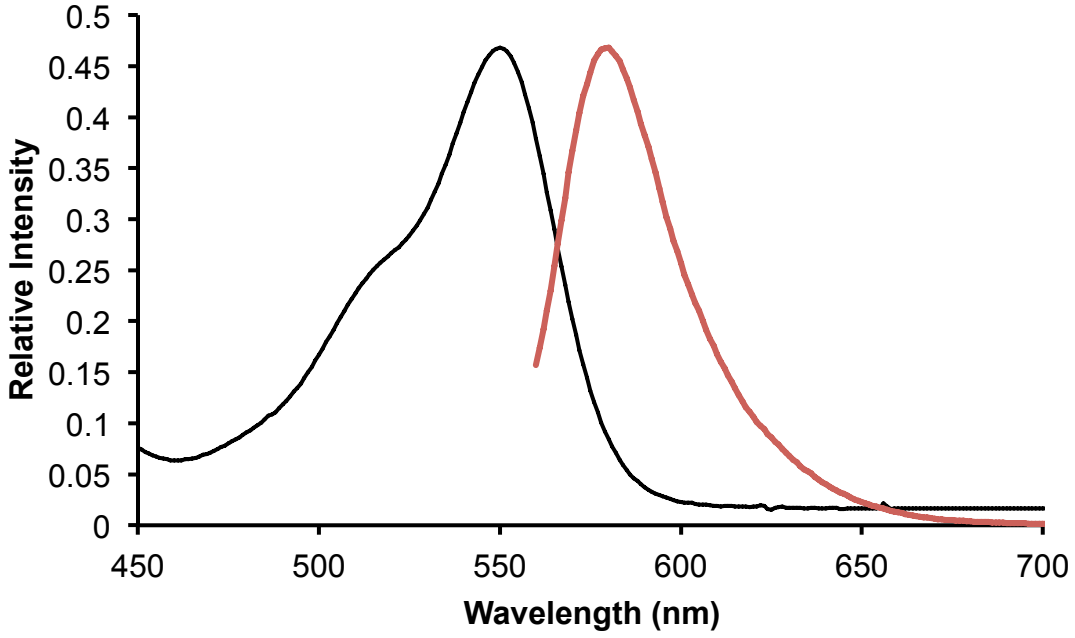
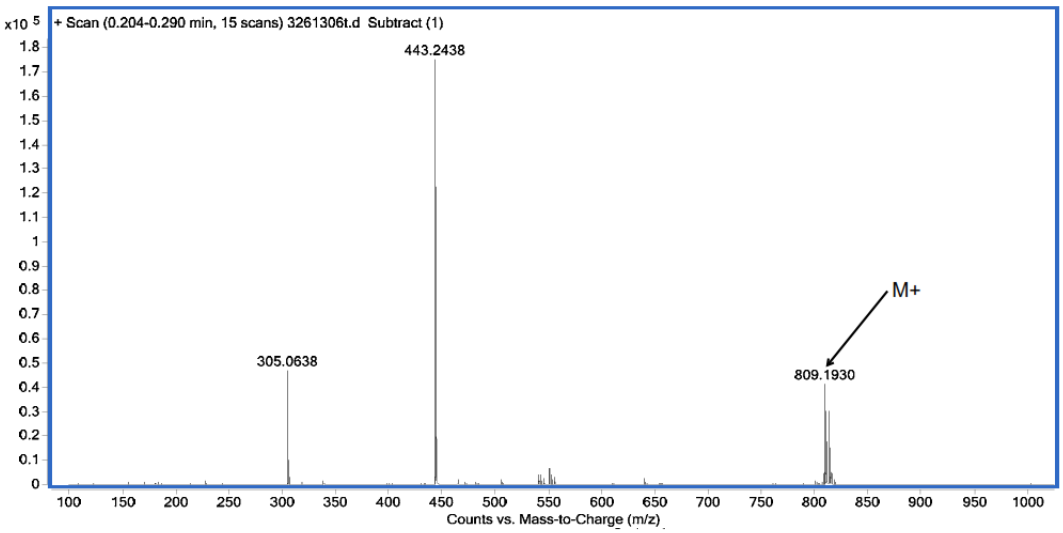
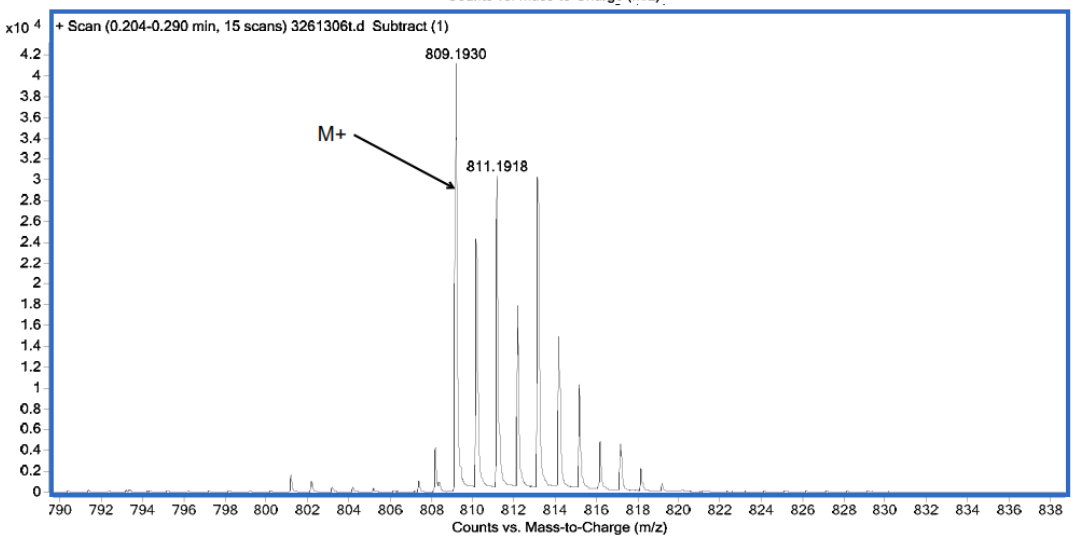


Figure S14. Overlay of the lowest energy absorption feature of **7** (black) with the emission spectrum (red) in acetonitrile.





Measured Mass 809.193

Element	Low Limit	High Limit
C	44	54
H	30	50
N	0	5
O	0	3
S	0	1
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C51 H39 N O3 S Zn	809.1937	-0.7	-0.8	33
C49 H37 N4 O2 S Zn	809.1923	0.7	0.8	33.5
C54 H35 N O3 Zn	809.1903	2.7	3.3	38
C54 H37 N2 S Zn	809.1963	-3.3	-4.1	37.5

Figure S15. ESI/APCI MS of **7**.

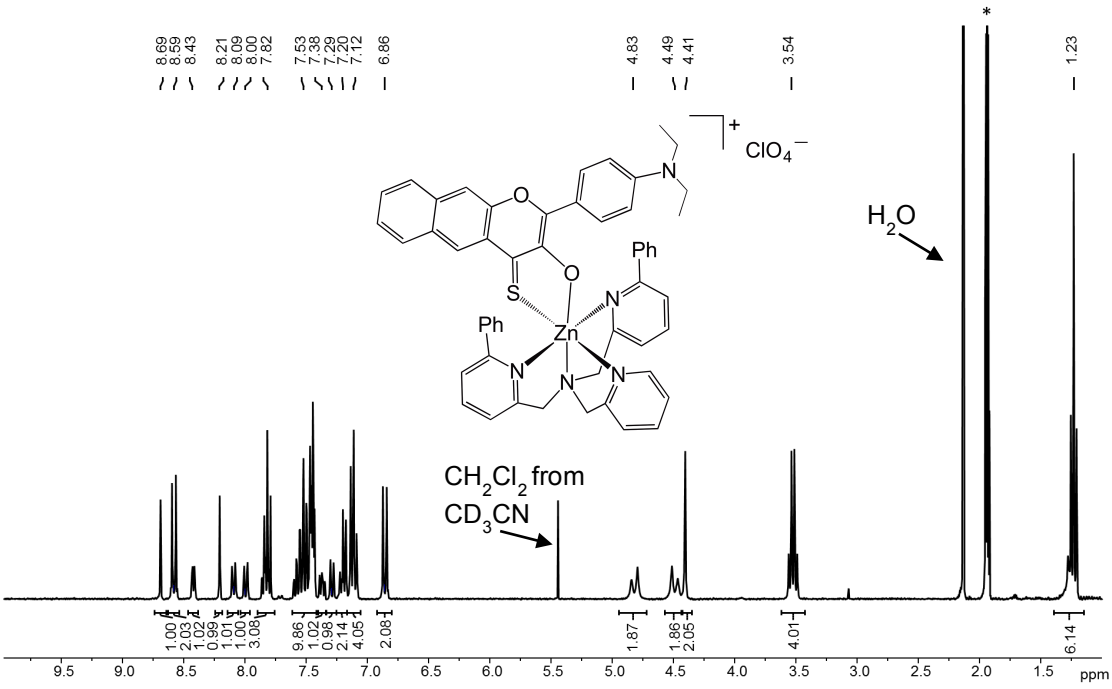


Figure S16. ^{1}H NMR of **8** in CD_3CN. (*denotes residual solvent)

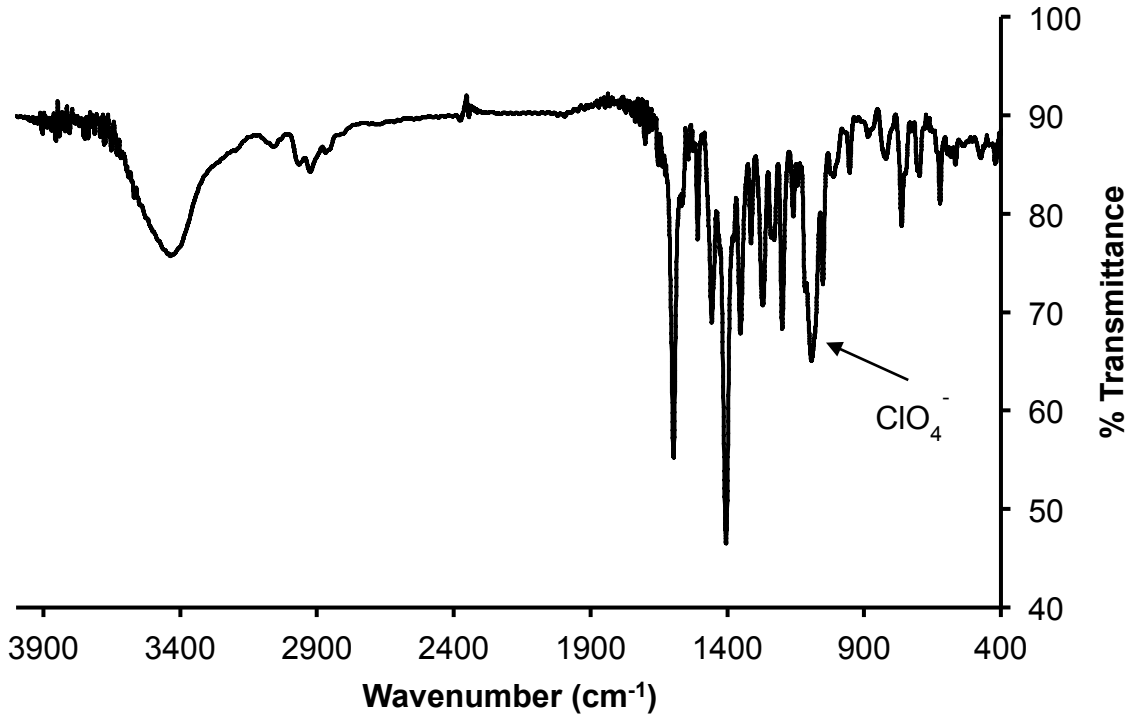


Figure S17. FT-IR of **8** in KBr.

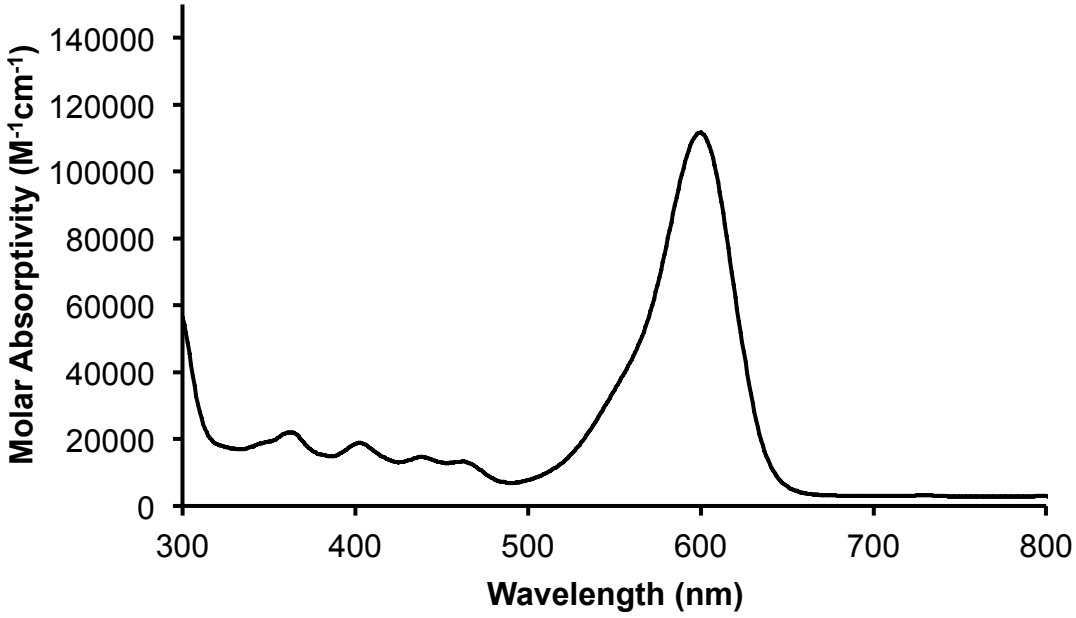


Figure S18. Absorption spectrum of **8** in acetonitrile.

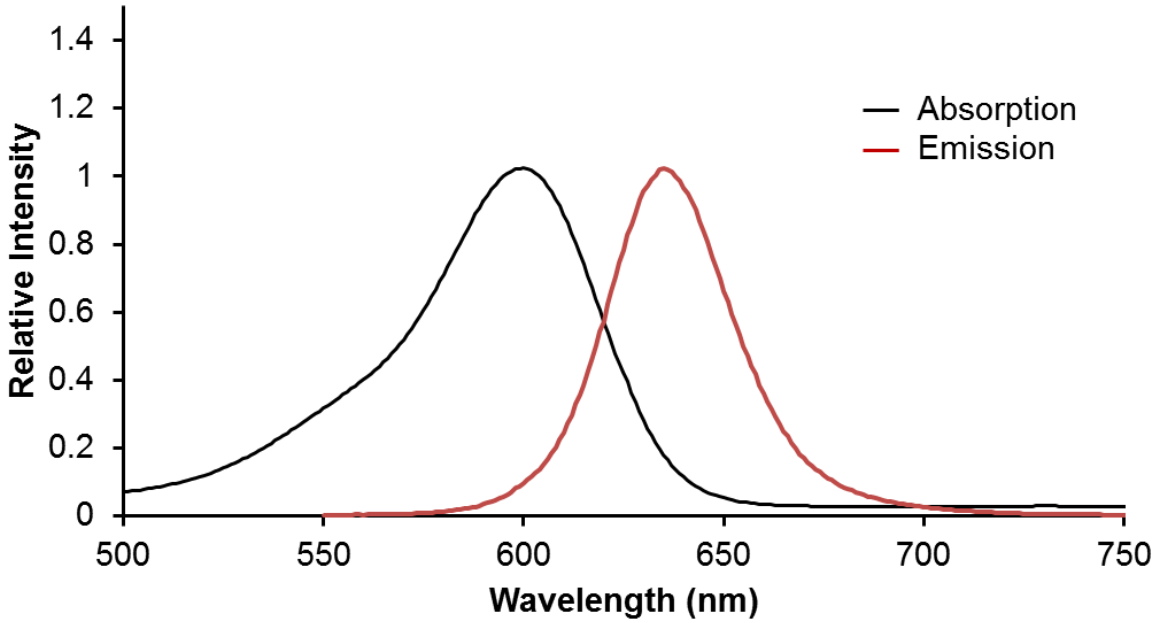
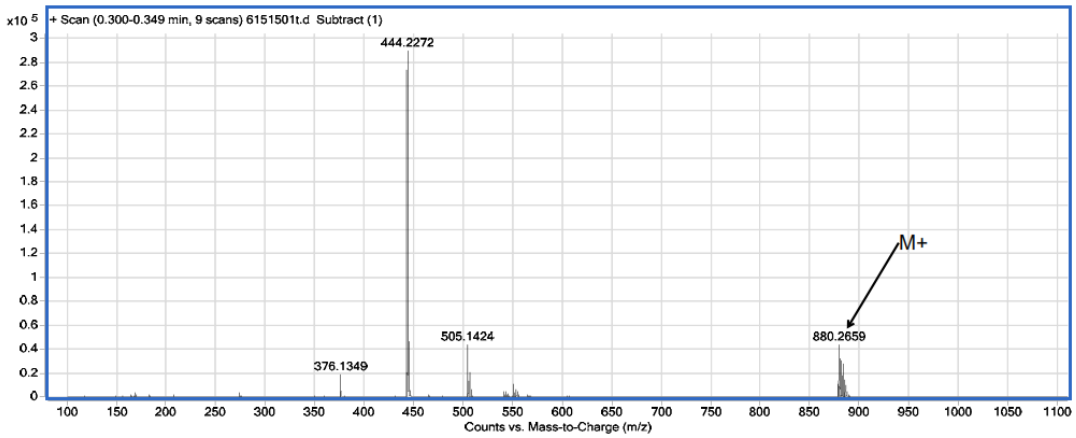
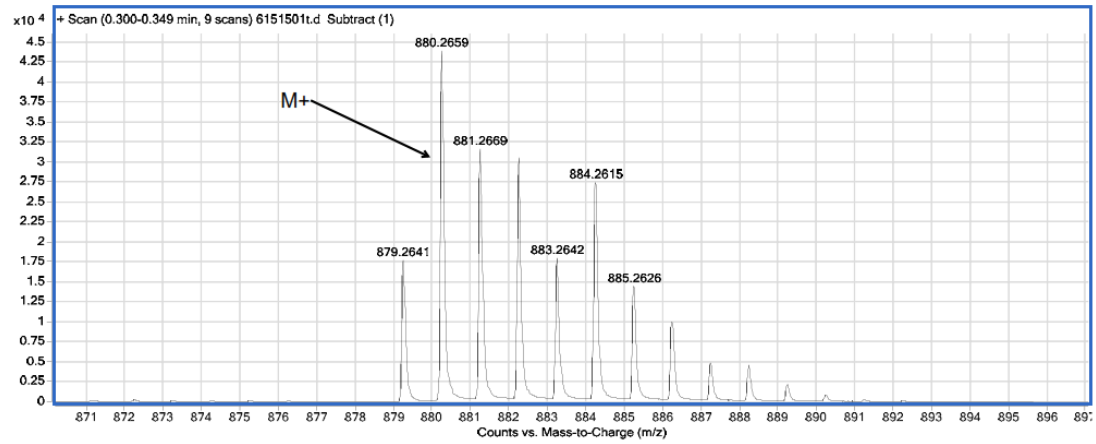


Figure S19. Overlay of the lowest energy absorption feature of **8** (black) with the emission spectrum (red) in acetonitrile.





Measured Mass	880.2659	
Element	Low Limit	High Limit
C	48	58
H	35	55
N	3	7
O	0	3
S	0	1
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C53 H46 N5 O2 S Zn	880.2658	0.1	0.1	33.5
C56 H42 N5 O2 Zn	880.2624	3.5	3.9	38.5
C58 H46 N3 S Zn	880.2698	-3.9	-4.5	37.5

Figure S20. ESI/APCI MS of **8**.

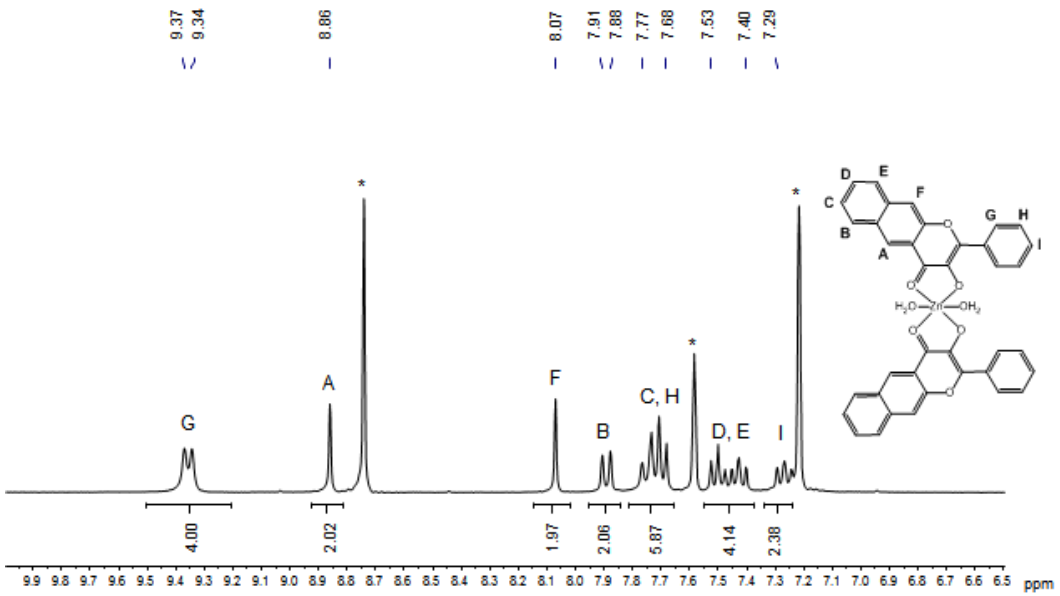


Figure S21. ^{1}H NMR of **9** in pyridine-d_5 (* indicates solvent peaks).

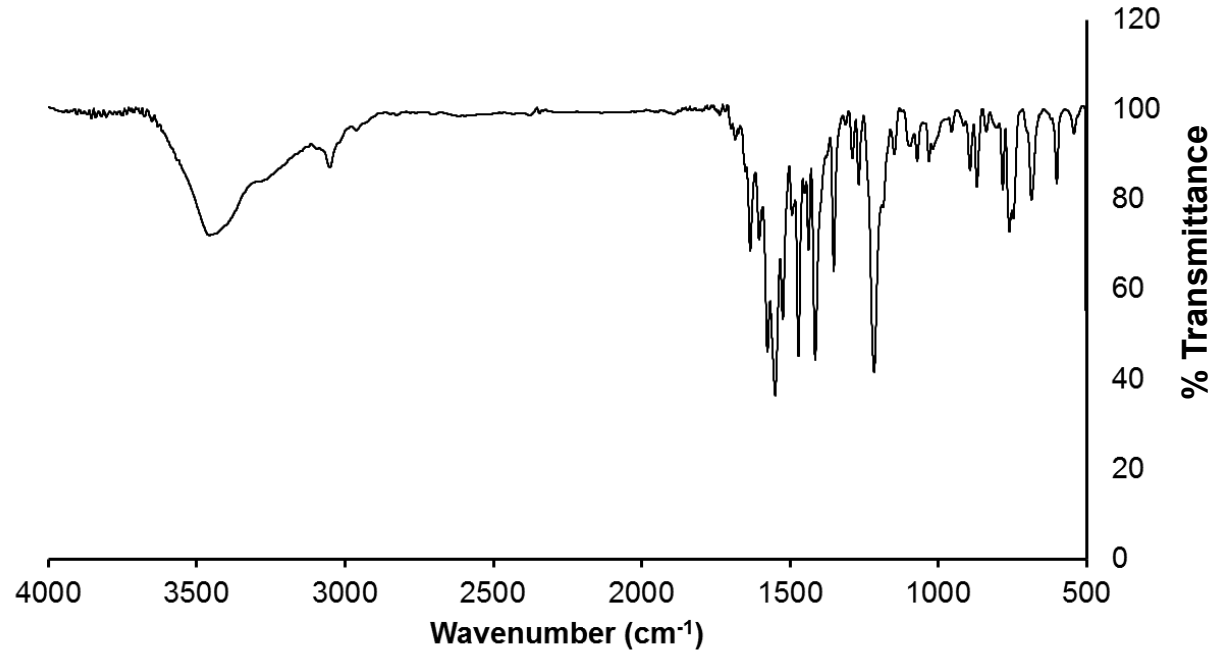


Figure S22. FTIR spectrum of **9**.

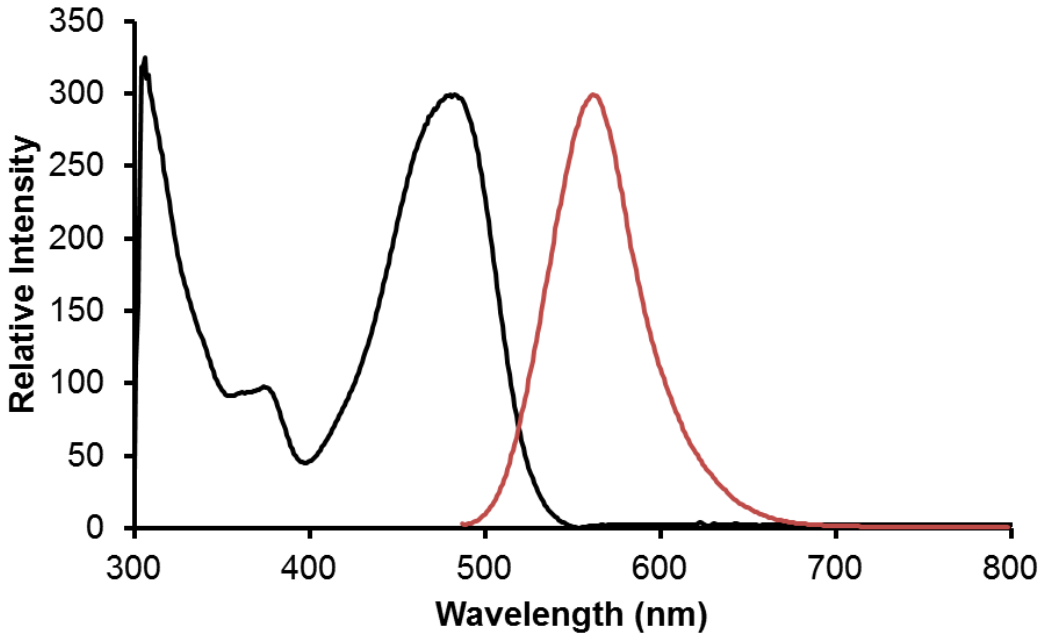
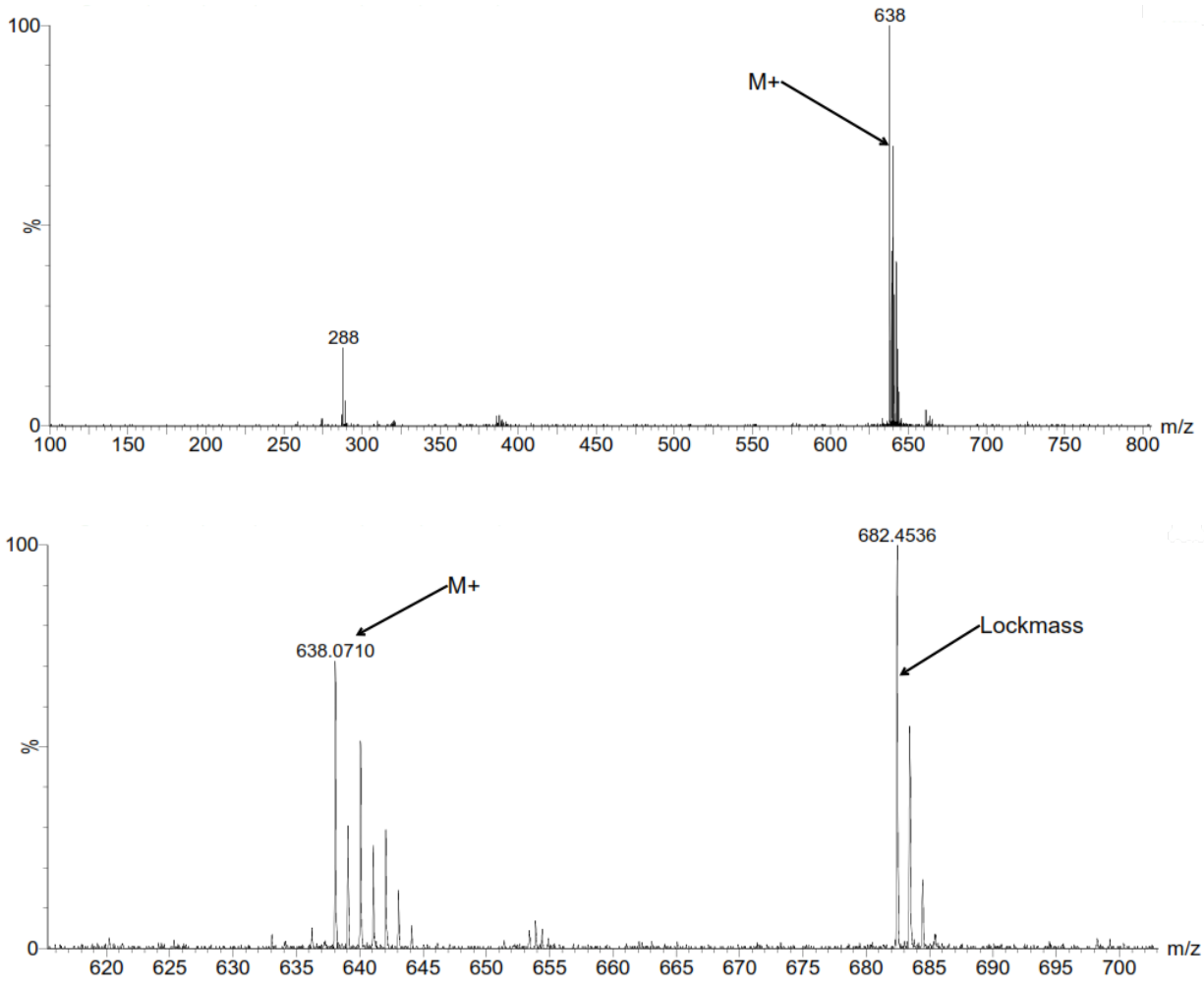


Figure S23. Absorption (black) and emission (red) spectra of **9**.



Measured Mass	638.071	
Element	Low Limit	High Limit
C	33	43
H	10	30
O	4	9
64Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C38 H22 O6 64Zn	638.0702	0.8	1.2	28

Figure S24. LIFDI-MS of **9.**

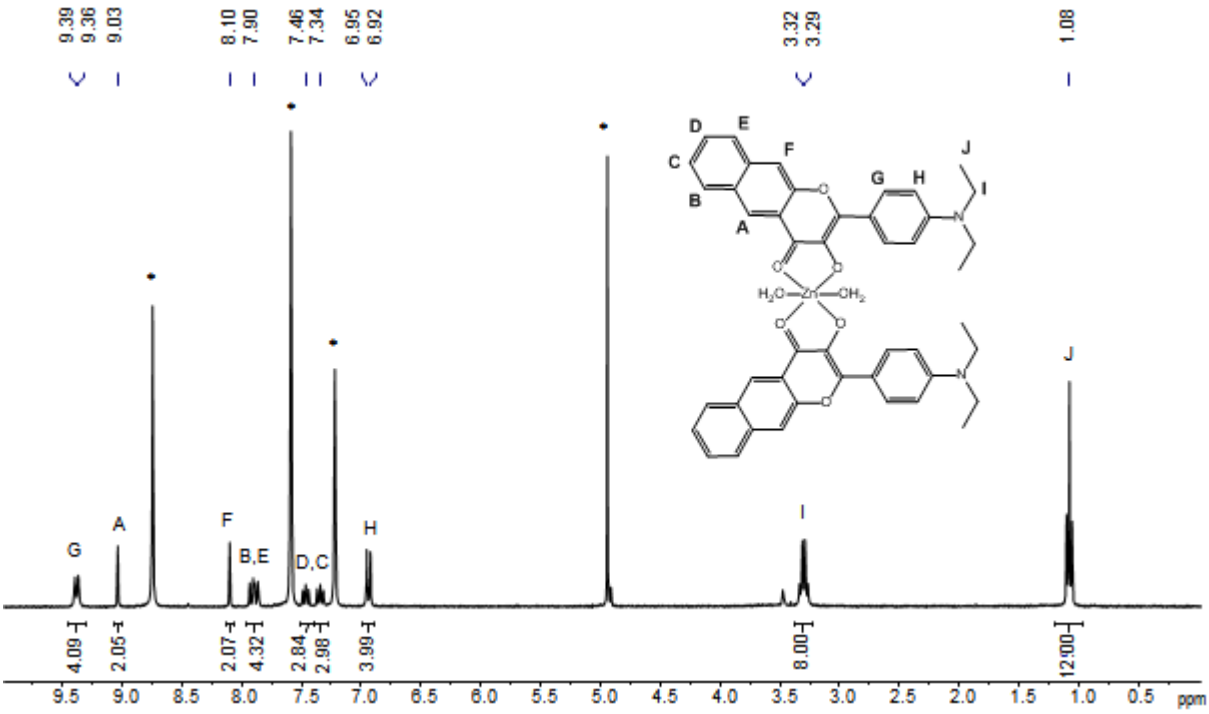


Figure S25. ^{1}H NMR of **10** in pyridine-d_5 (* denotes residual solvent peaks).

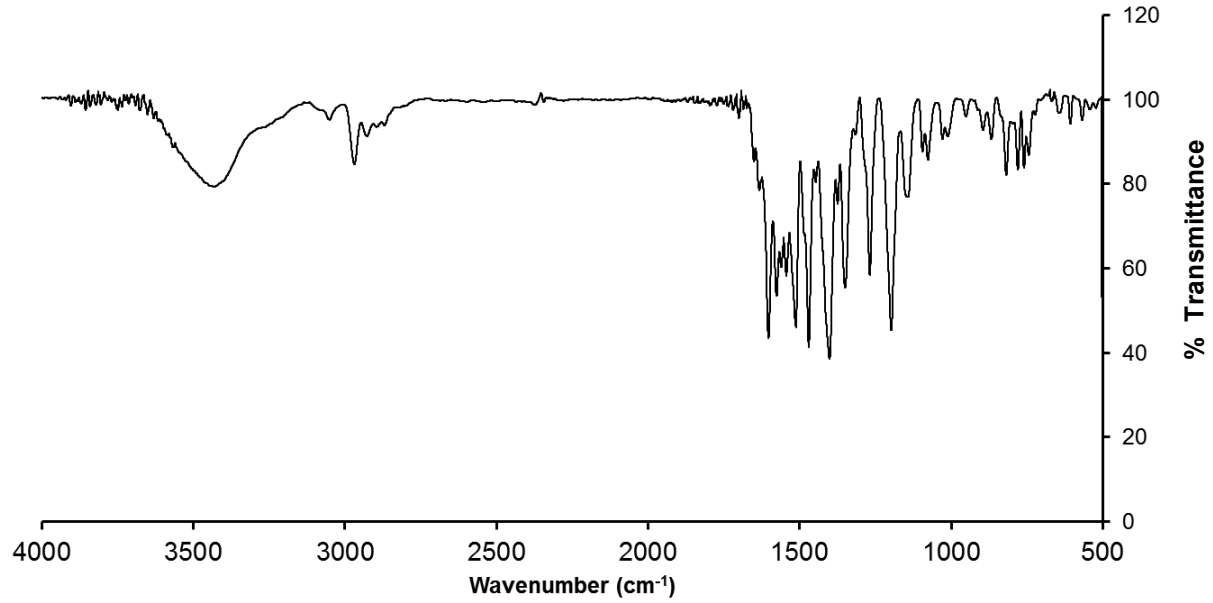


Figure S26. FTIR spectrum of **10**.

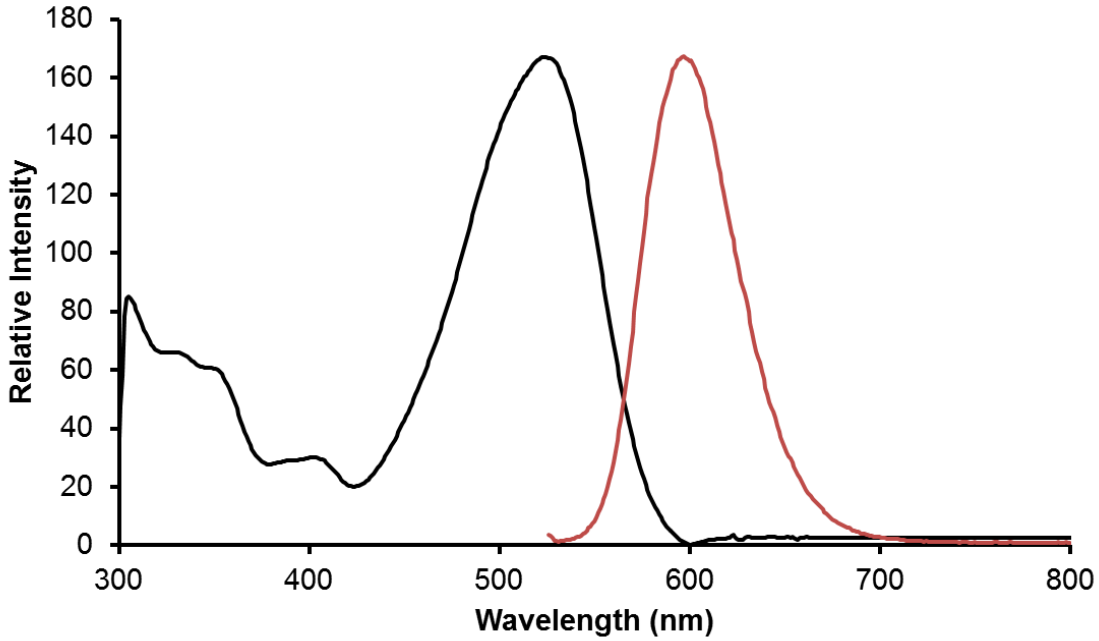
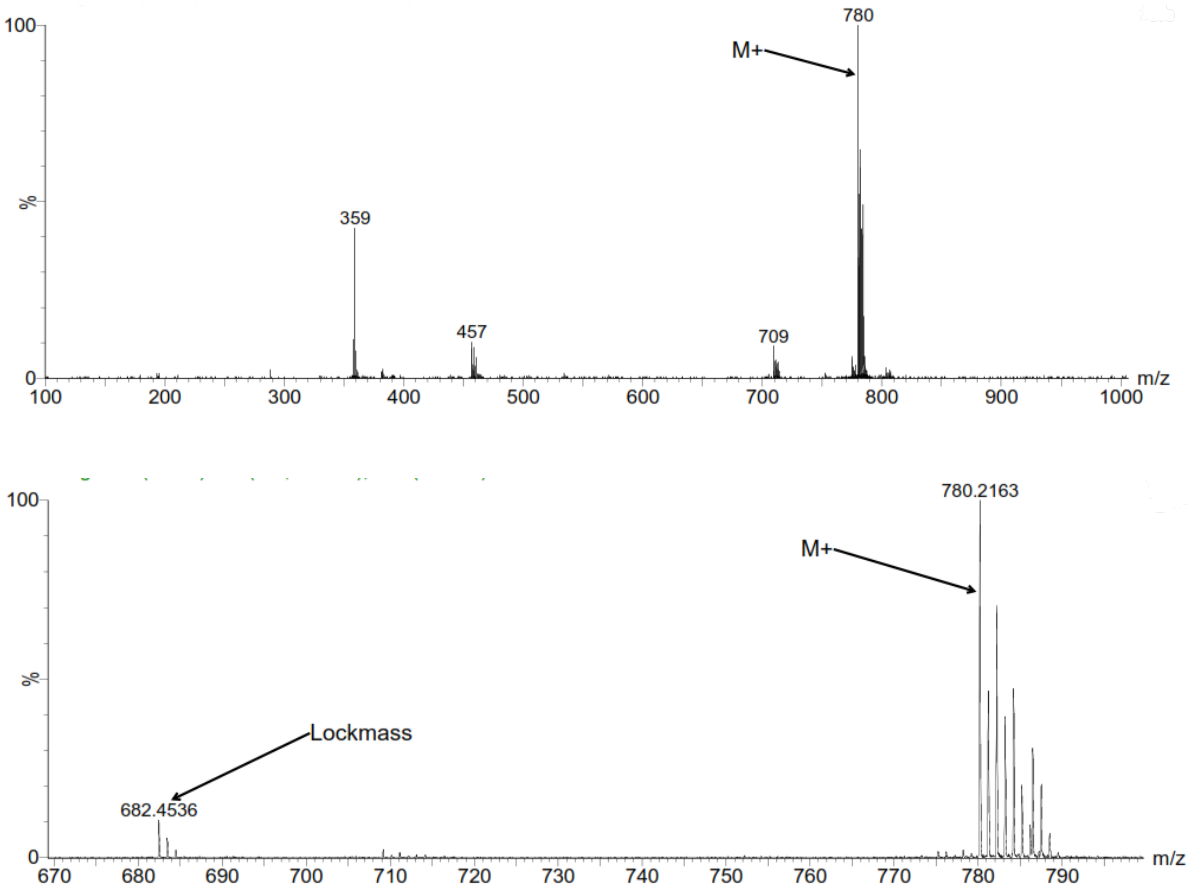


Figure S27. Absorption (black) and emission (red) spectra of **10**.



Measured Mass	780.2163	
Element	Low Limit	High Limit
C	41	51
H	30	50
N	0	2
O	4	8
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C46 H40 N2 O6 Zn	780.2172	-0.9	-1.2	28

Figure S28. LIFDI-MS of **10**.

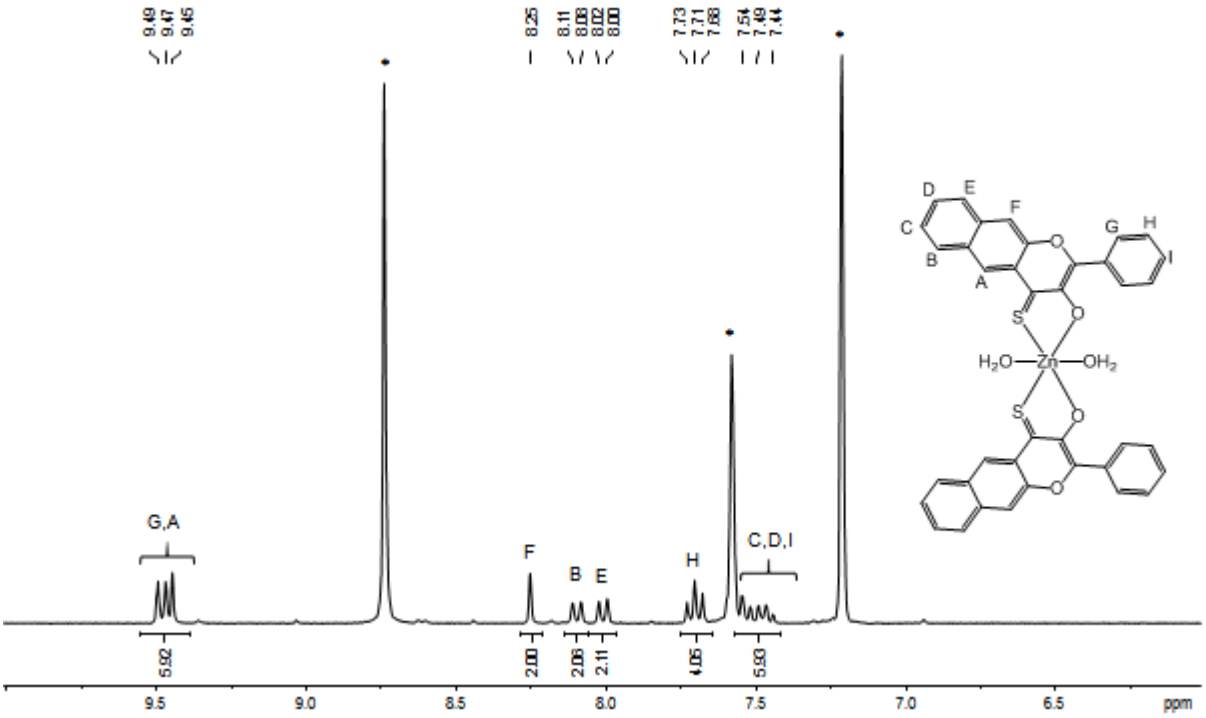


Figure S29. ^{1}H NMR of **11** in pyridine-d_5 (* denotes residual solvent peaks).

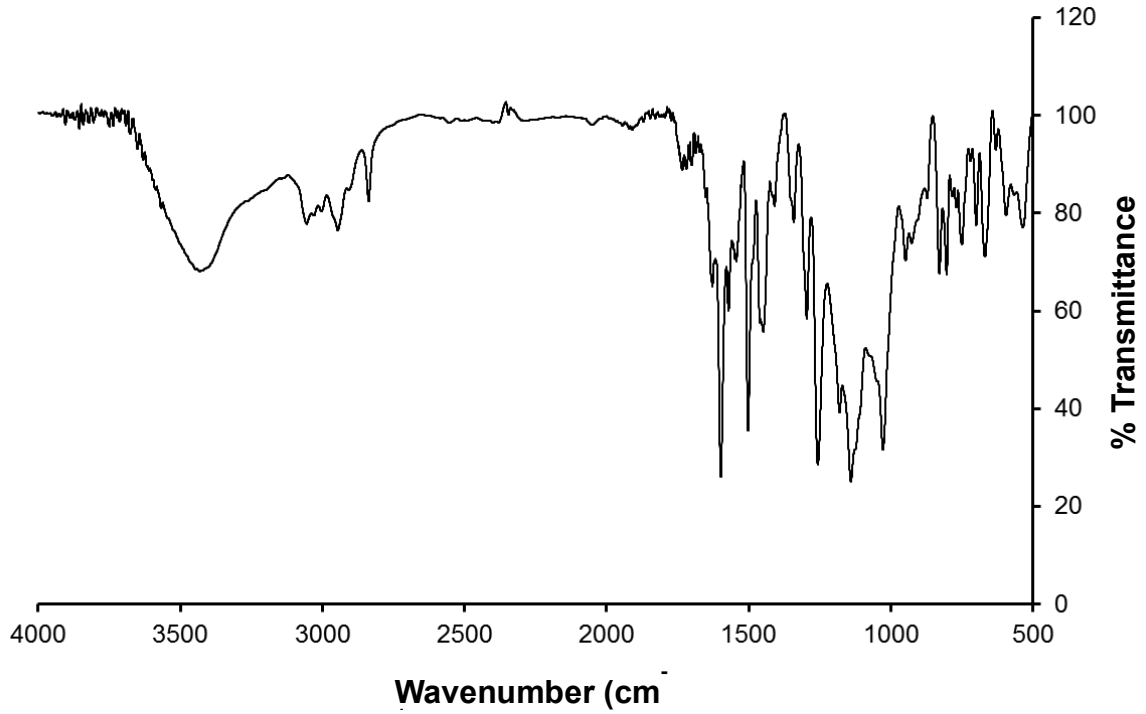


Figure S30. FTIR spectrum of **11**.

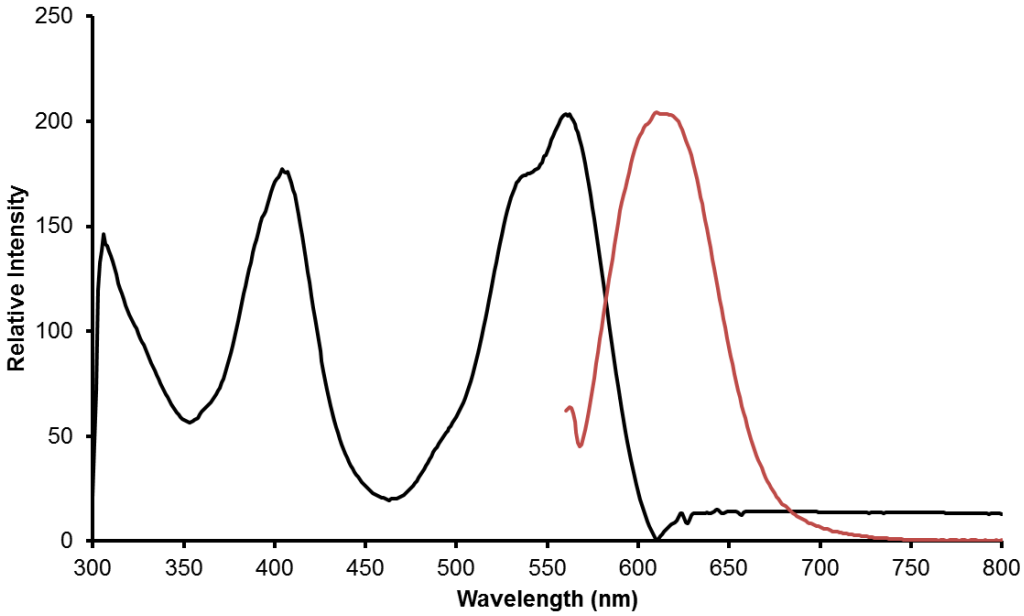
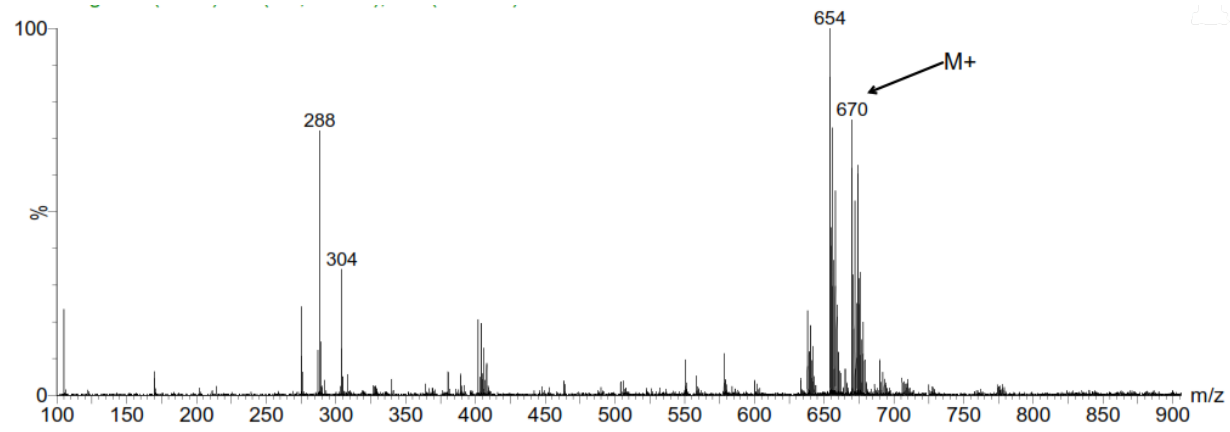
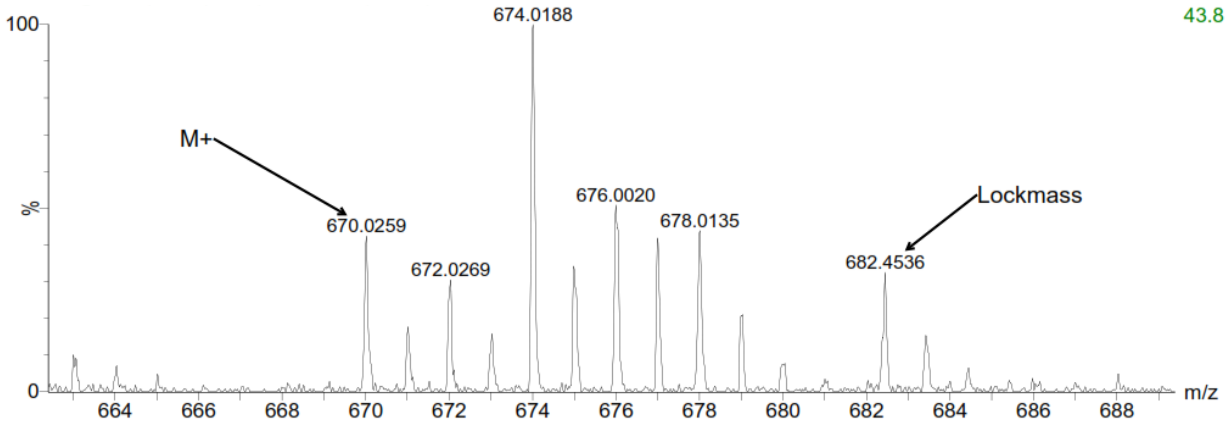


Figure S31. Absorption (black) and emission (red) spectra of **11**.





Measured Mass	670.0259	
Element	**Low Limit**	**High Limit**
C	33	43
H	15	35
S	0	2
O	2	6
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C38 H22 O4 S2 Zn	670.0246	1.4	2.0	28

Figure S32. LIFDI-MS of **11**.

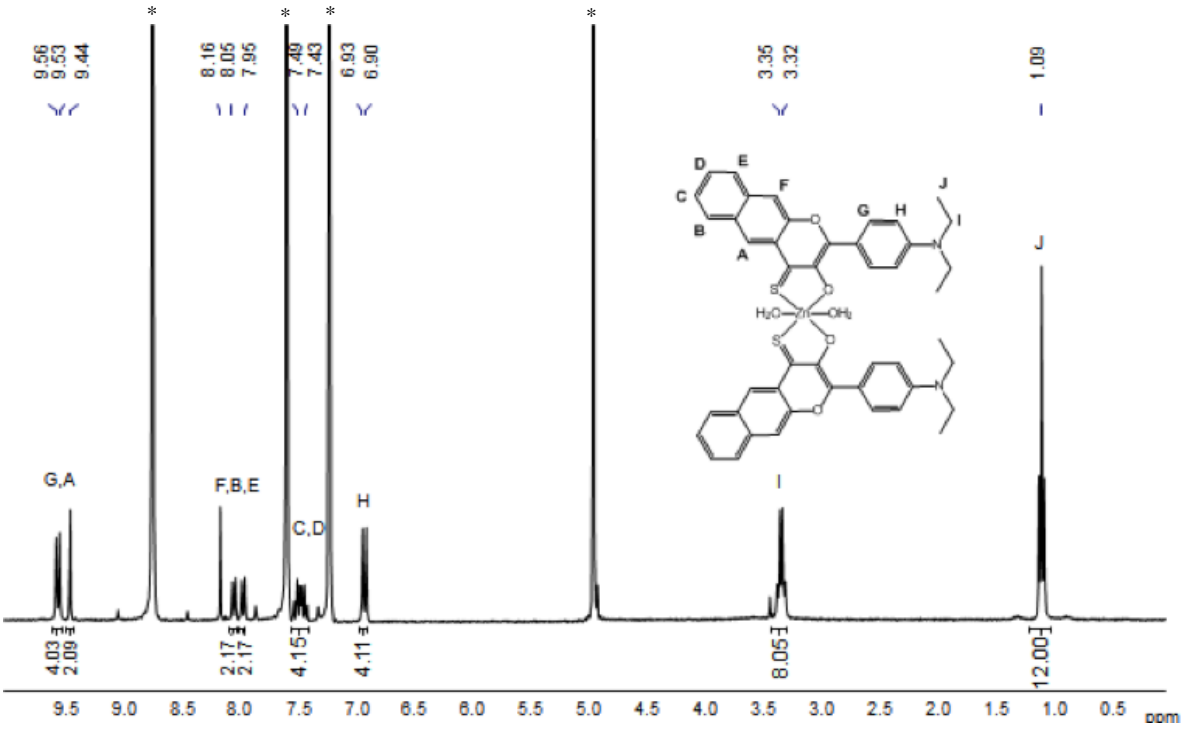


Figure S33. ^{1}H NMR of **12** in pyridine-d_5 (* denotes residual solvent peaks).

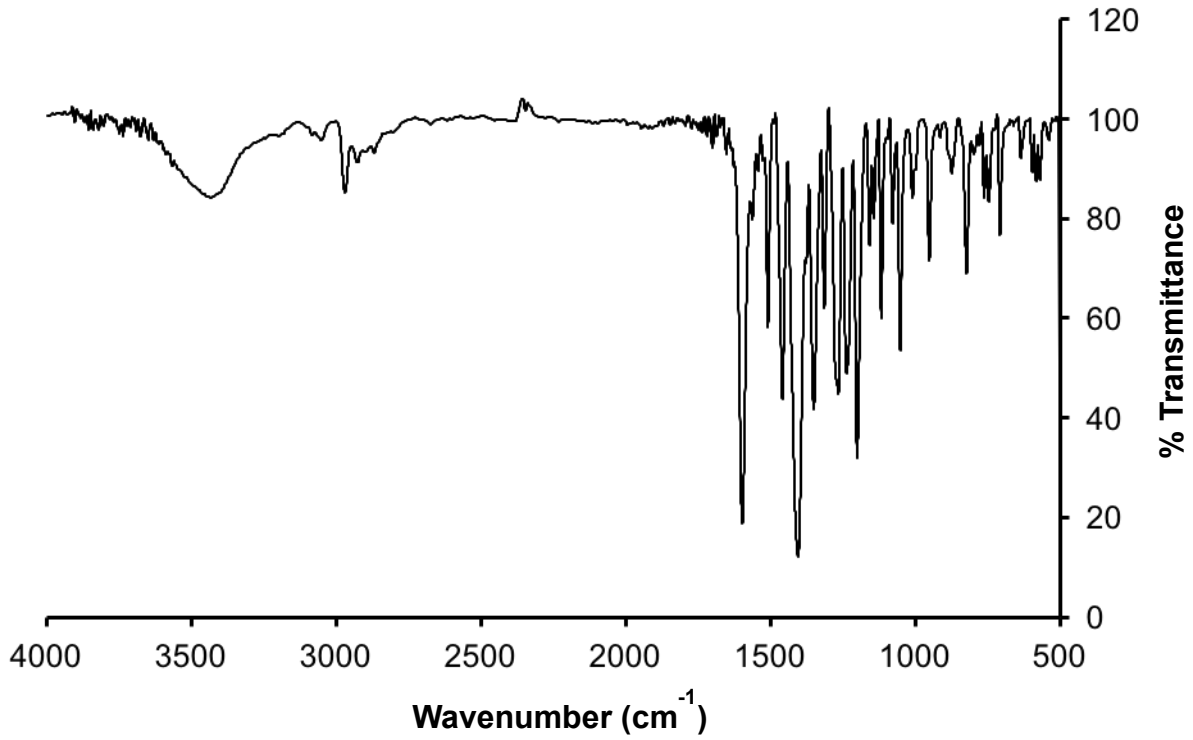


Figure S34. FTIR spectrum of **12**.

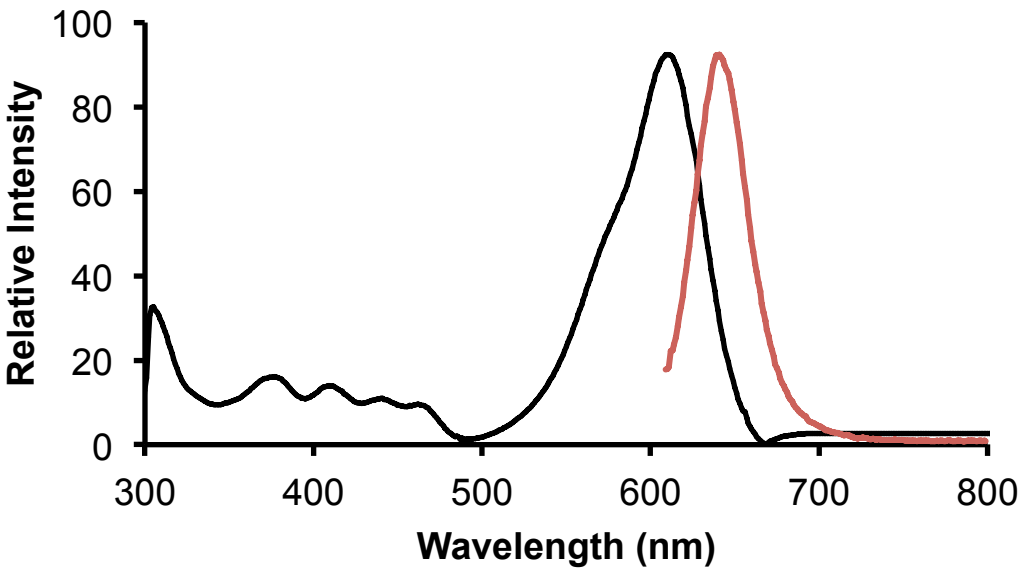
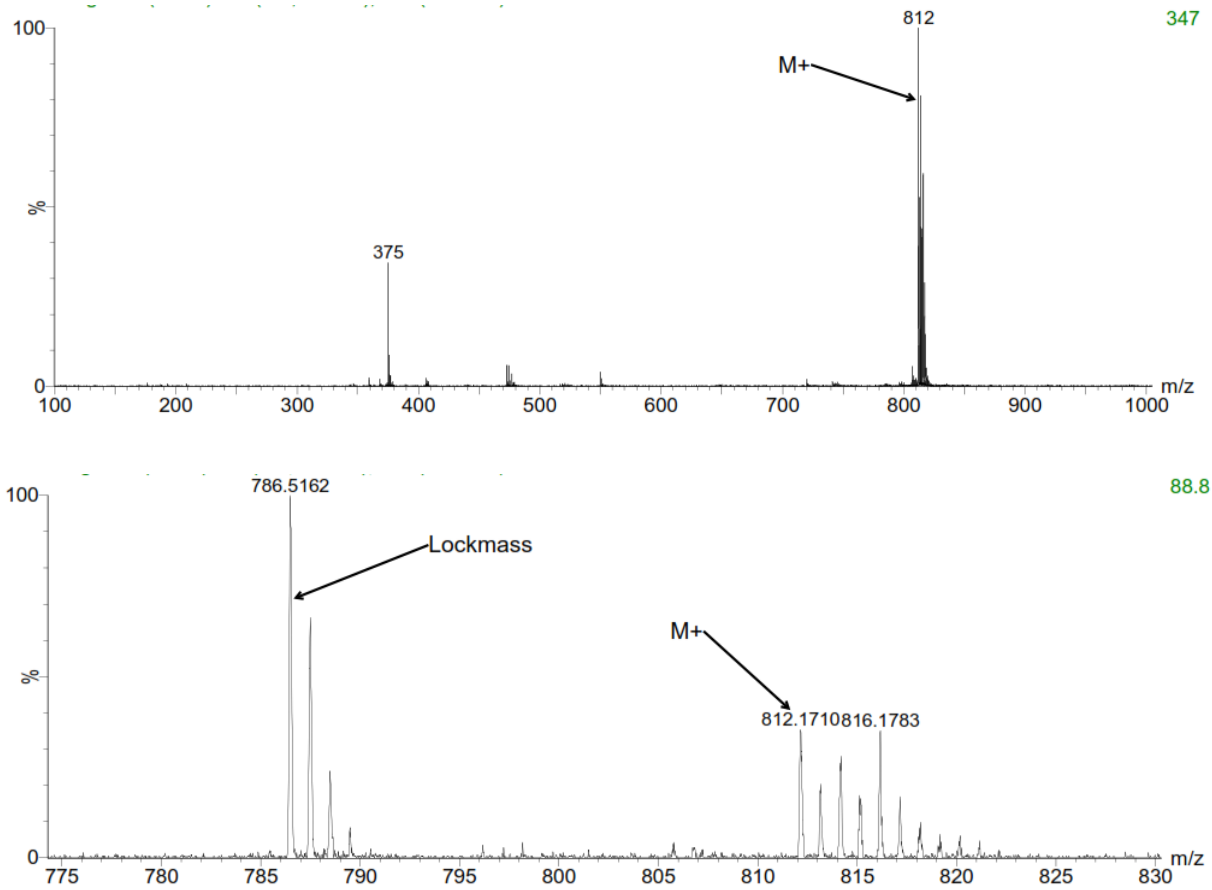


Figure S35. Absorption (black) and emission (red) spectra of **12**.



Measured Mass	812.171	
Element	**Low Limit**	**High Limit**
C	41	51
H	30	50
N	0	2
O	2	6
S	0	2
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C46 H40 N2 O4 S2 Zn	812.1715	-0.5	-0.7	28
C49 H36 N2 O4 S Zn	812.1682	2.8	3.5	33

Figure S36. LIFDI-MS of **12**.

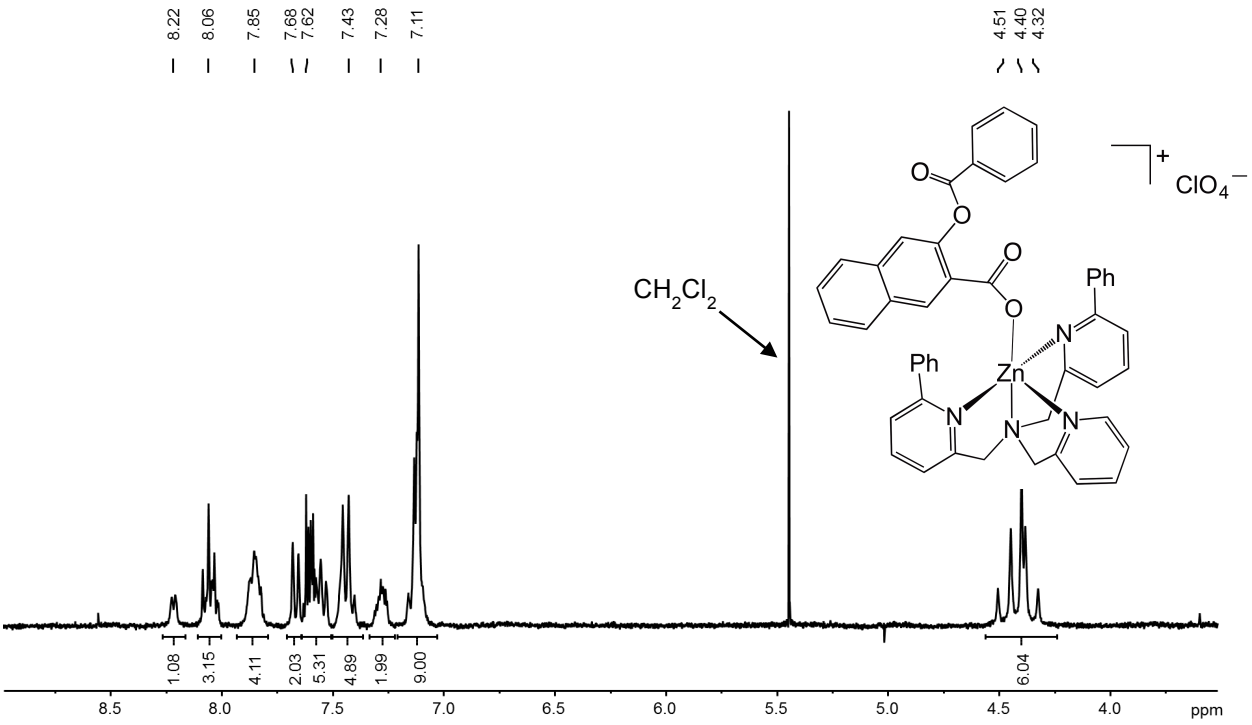


Figure S37. ^{1}H NMR of **13** in CD_3CN.

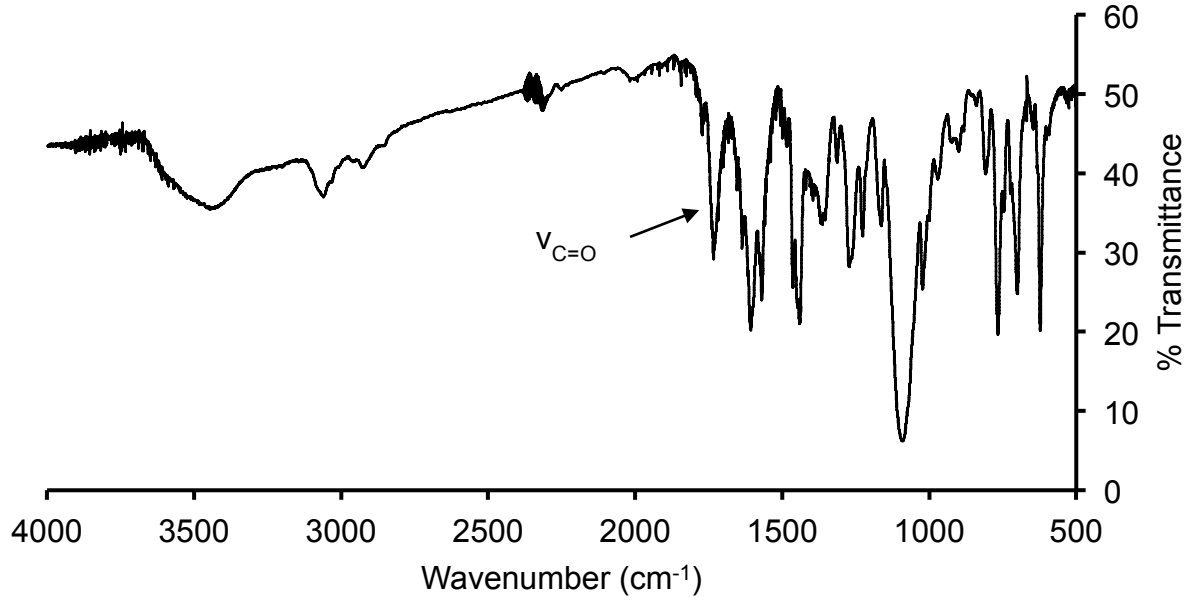
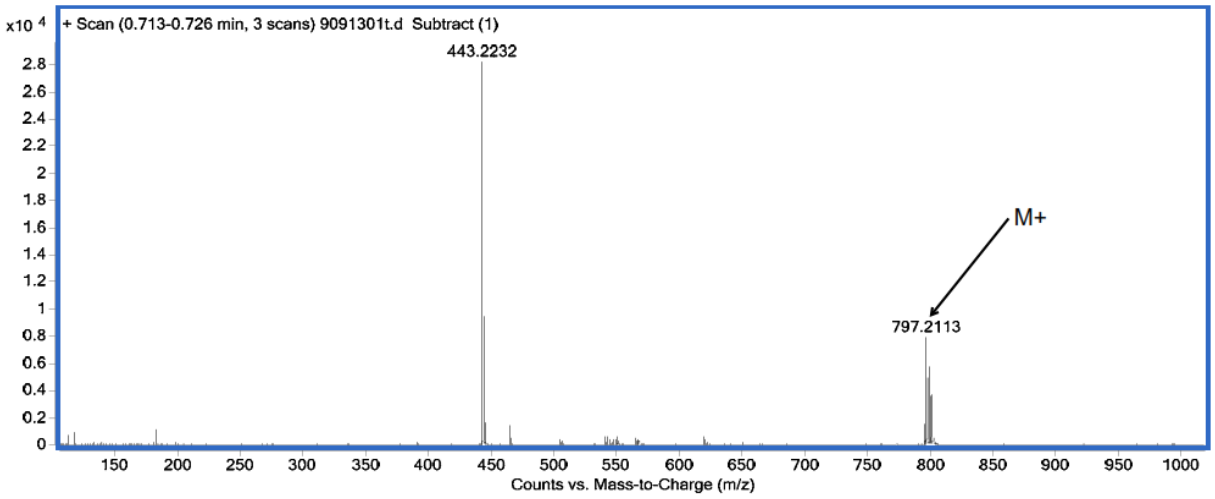
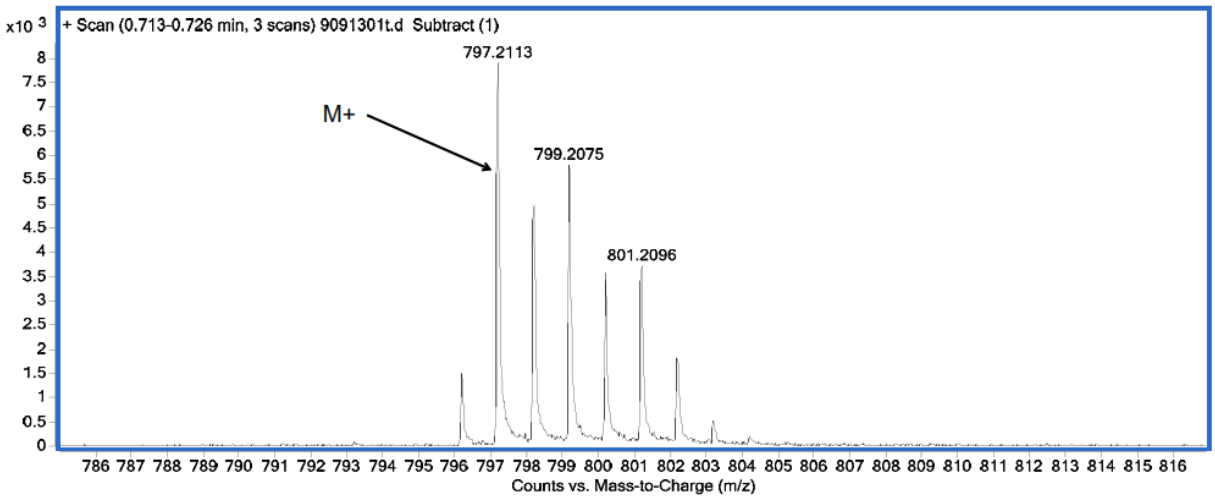


Figure S38. FT-IR of **13** in KBr.

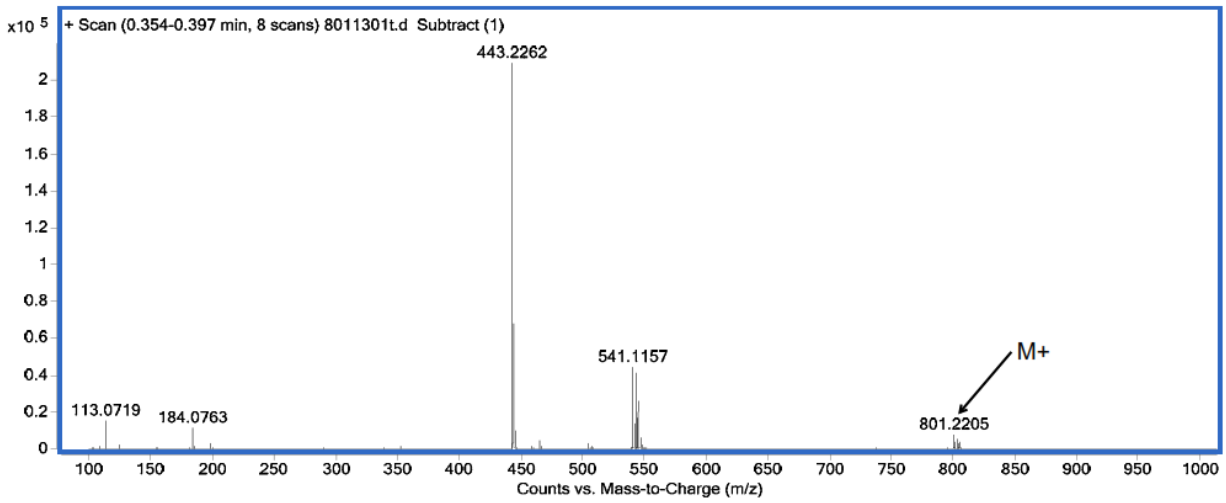


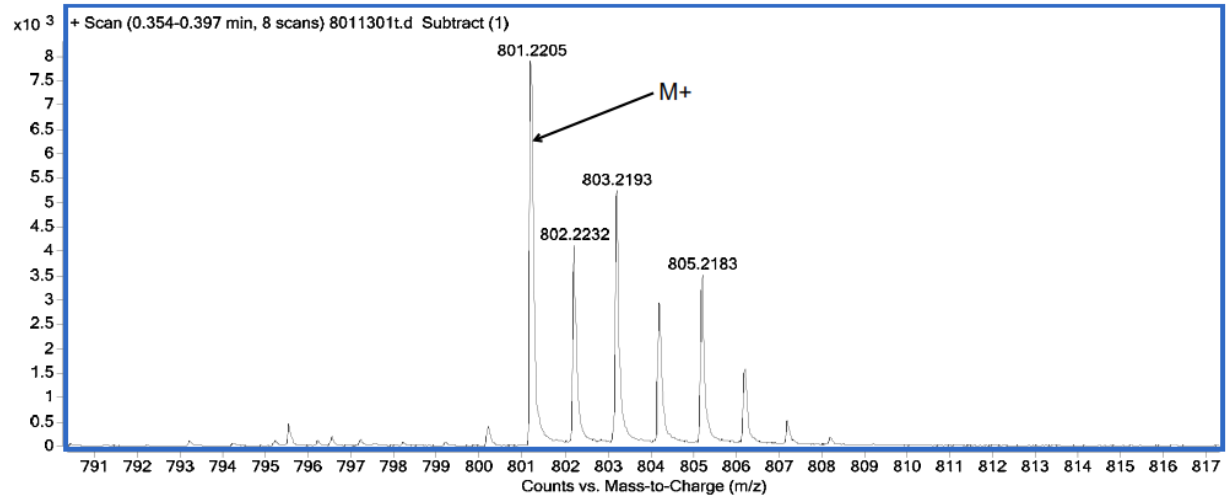


Measured Mass	797.2113	
Element	Low Limit	High Limit
C	43	53
H	30	50
N	2	6
O	2	6
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C48 H37 N4 O4 Zn	797.2101	1.2	1.5	32.5
C53 H37 N2 O2 Zn	797.2141	-2.8	-3.5	36.5

Figure S39. ESI/APCI MS of **13**.





Measured Mass 801.2205

Element	Low Limit	High Limit
C	43	53
H	30	50
N	0	5
O	0	2
18O	0	2
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C51 H37 N4 O2 Zn	801.2202	0.3	0.3	35.5
C52 H37 N3 O 18O Zn	801.2214	-0.9	-1.1	36
C48 H37 N4 O2 18O2 Zn	801.2186	1.9	2.4	32.5
C53 H37 N2 18O2 Zn	801.2226	-2.1	-2.6	36.5

Figure S40. ESI/APCI MS of **13** demonstrating $^{18}O_2$ incorporation.

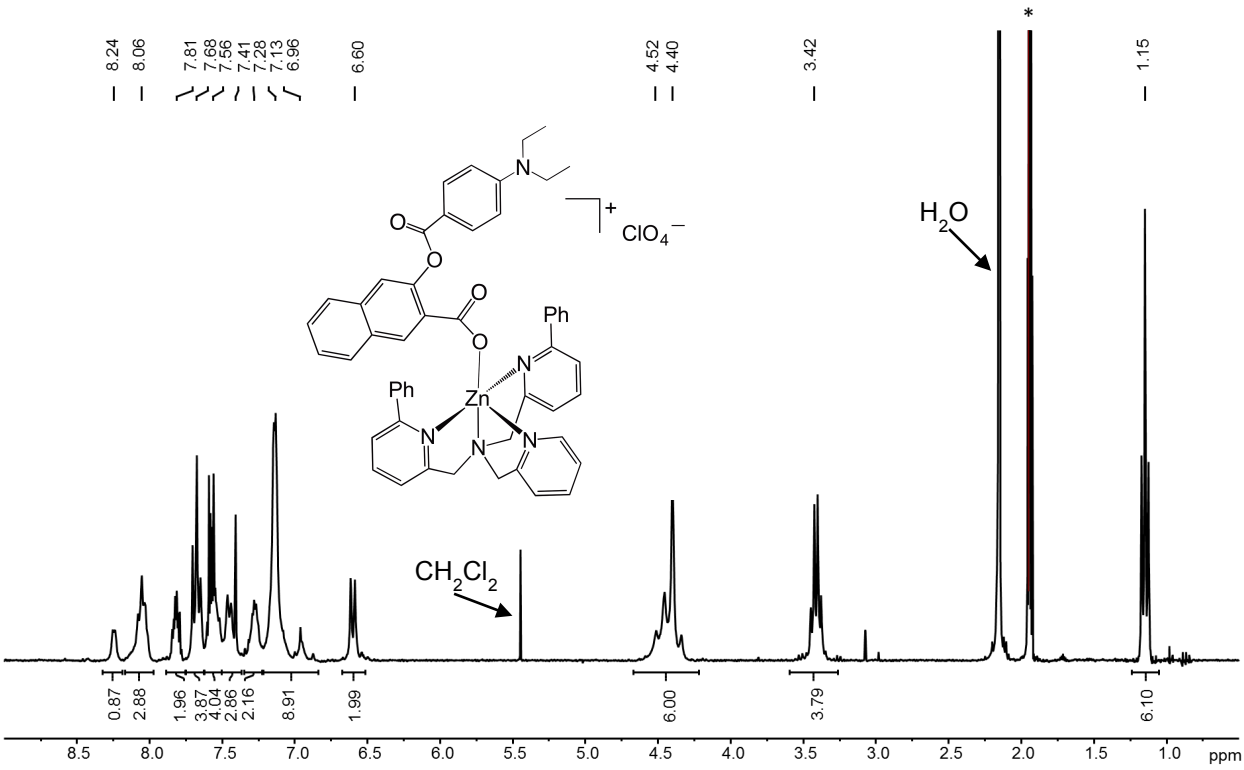


Figure S41. ^{1}H NMR of **14** in CD_3CN. (*denotes residual solvent)

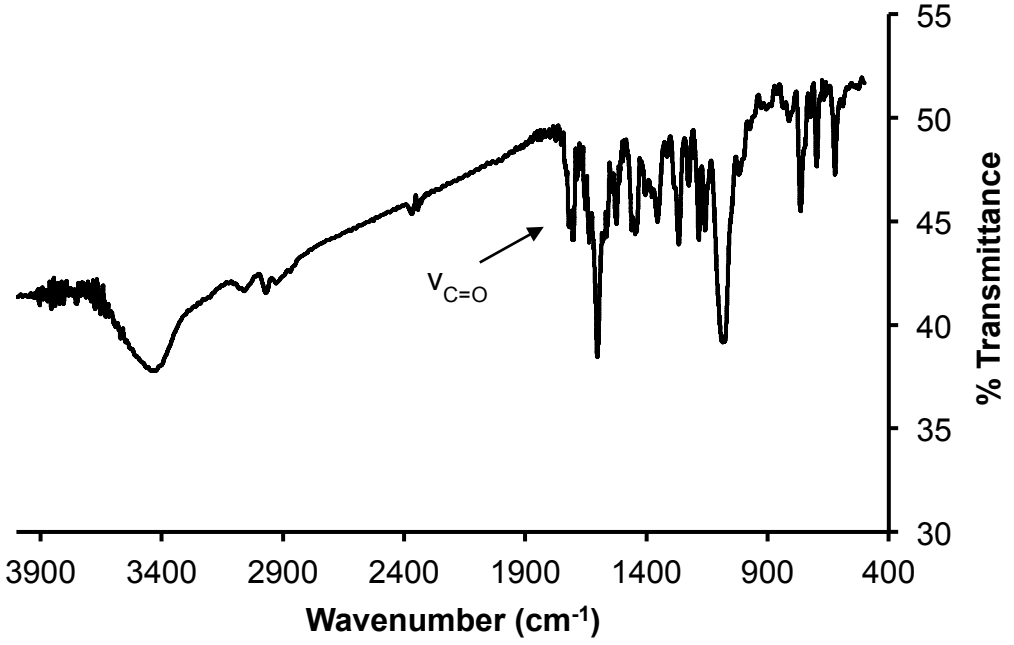
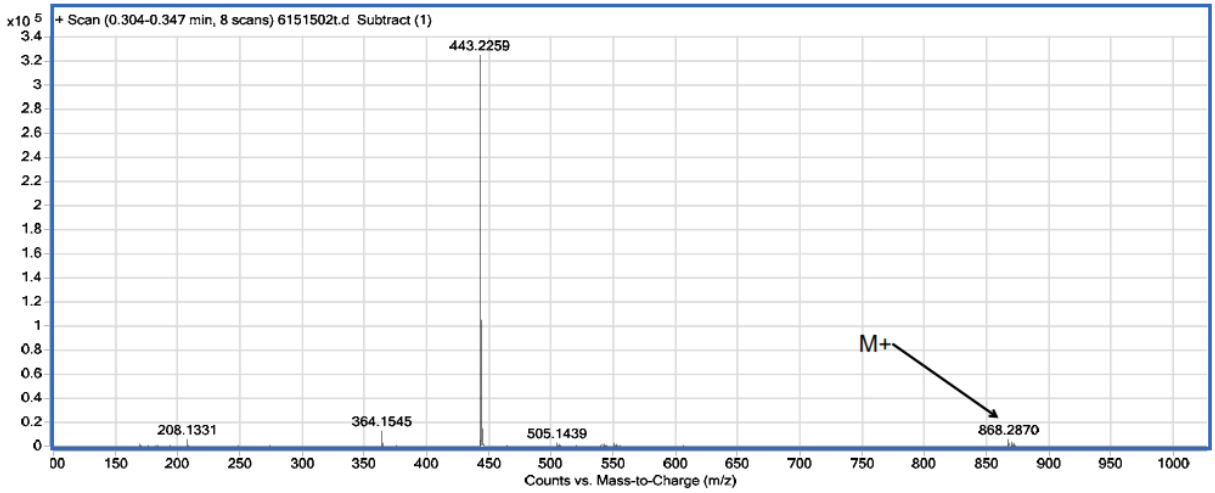
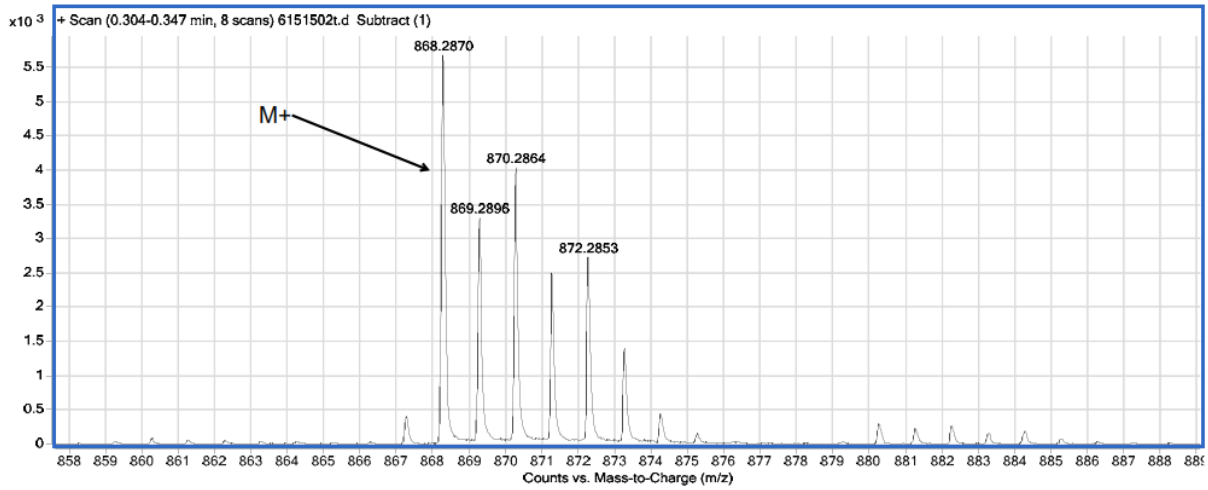


Figure S42. FT-IR of **14** in KBr.





Measured Mass 868.287

Element	Low Limit	High Limit
C	48	58
H	35	55
N	3	7
O	2	6
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C57 H46 N3 O2 Zn	868.2876	-0.6	-0.7	36.5
C53 H38 N7 O6	868.2878	-0.8	-0.9	38.5
C52 H46 N5 O4 Zn	868.2836	3.4	3.9	32.5

Figure S43. ESI/APCI MS of **14**.

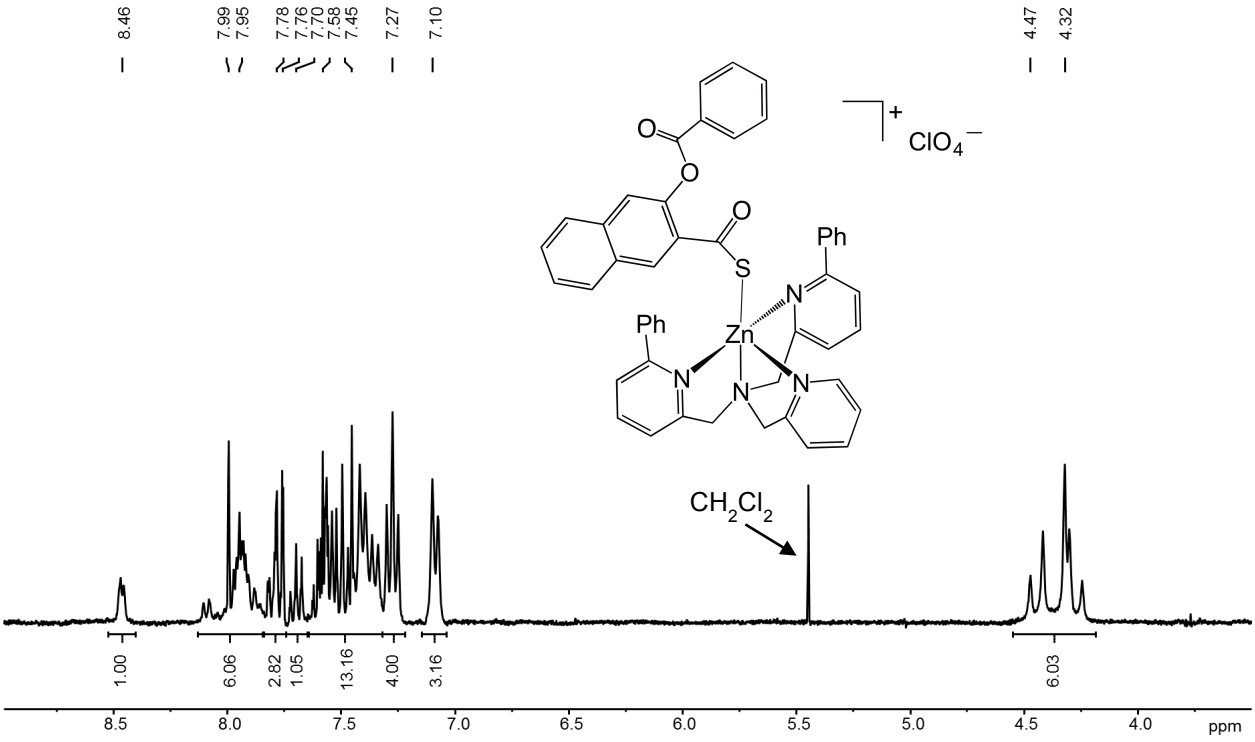


Figure S44. ^{1}H NMR of **15** in CD_3CN.

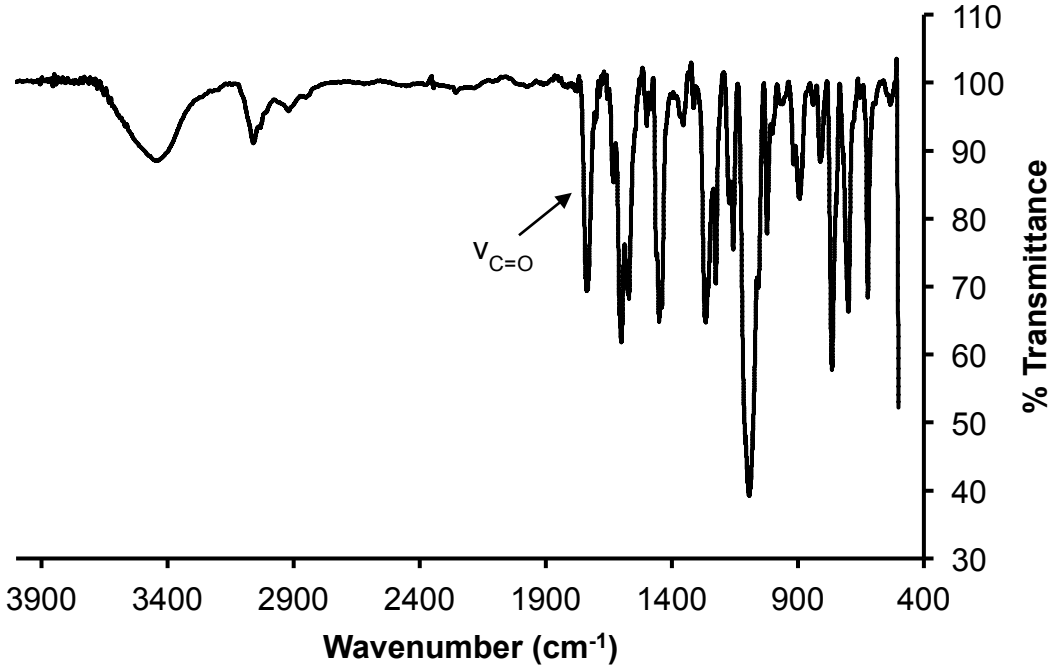
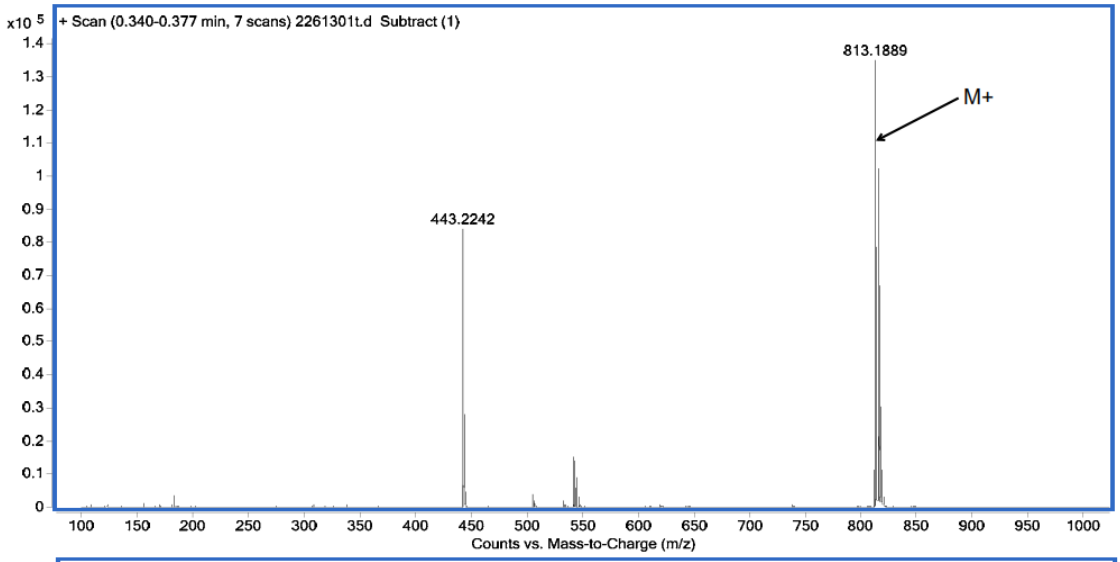
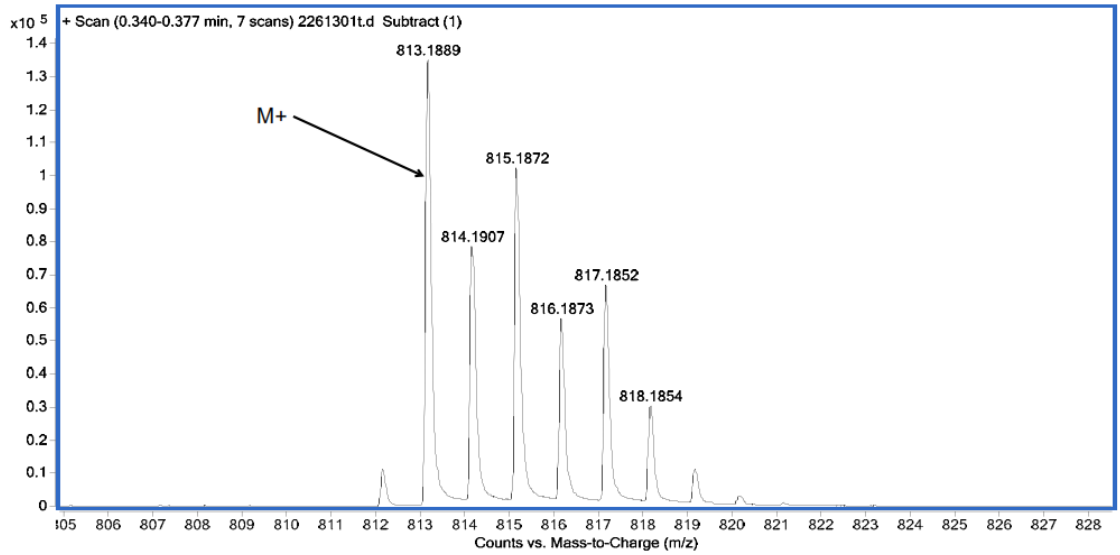


Figure S45. FT-IR of **15** in KBr.





Measured Mass 813.1889

Element	Low Limit	High Limit
C	43	53
H	30	50
N	2	6
O	1	5
S	0	1
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C48 H37 N4 O3 S Zn	813.1872	1.7	2.0	32.5
C53 H37 N2 O S Zn	813.1913	-2.4	-2.9	36.5
C47 H35 N5 O5 Zn	813.1924	-3.5	-4.3	33

Figure S46. ESI/APCI MS of **15**.

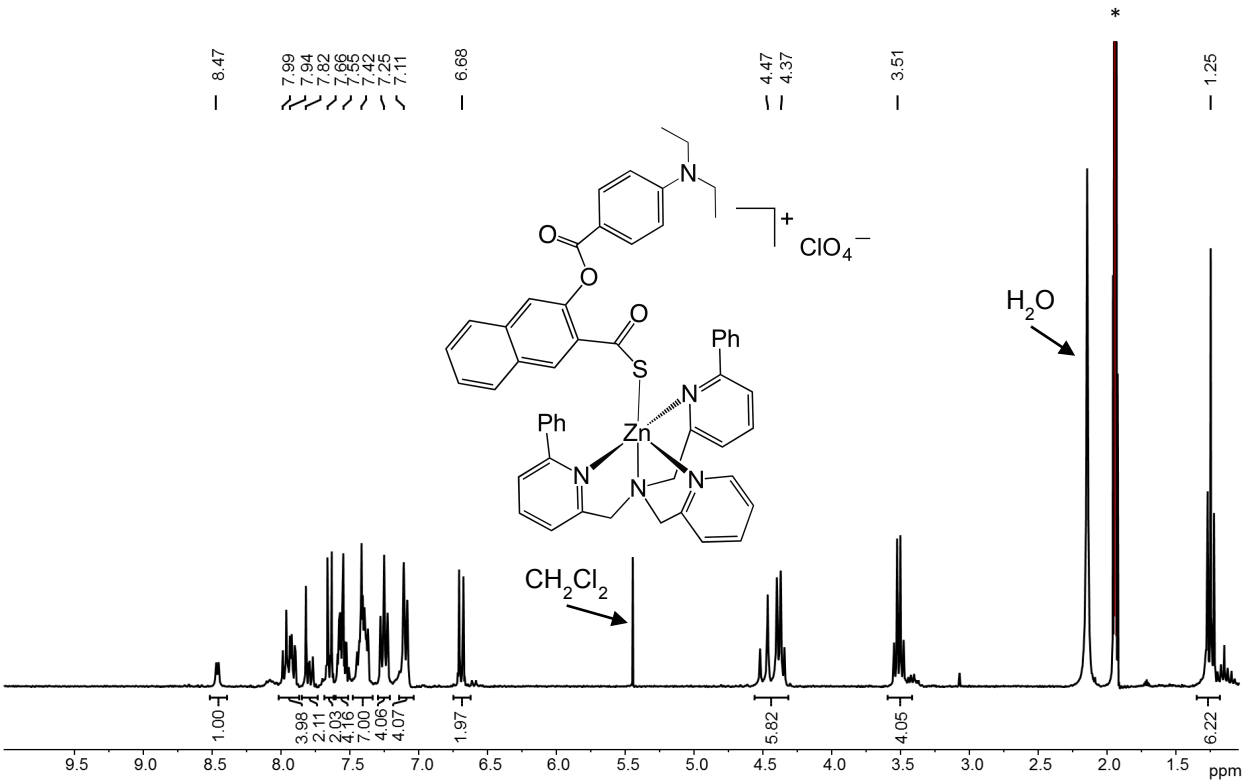


Figure S47. ^{1}H NMR of **16** in CD_3CN. (*denotes residual solvent)

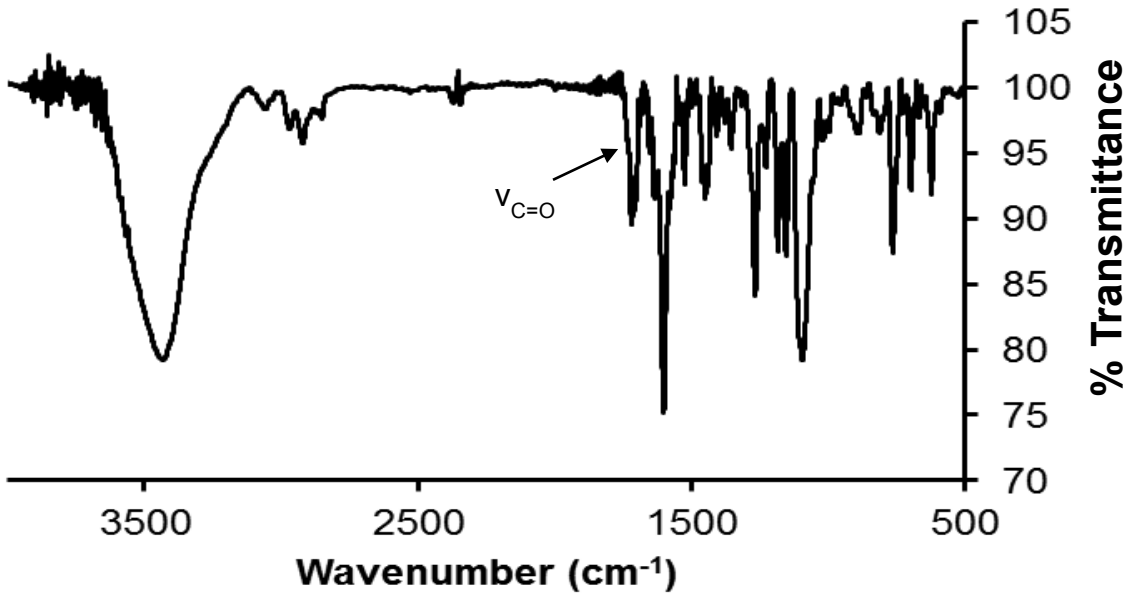
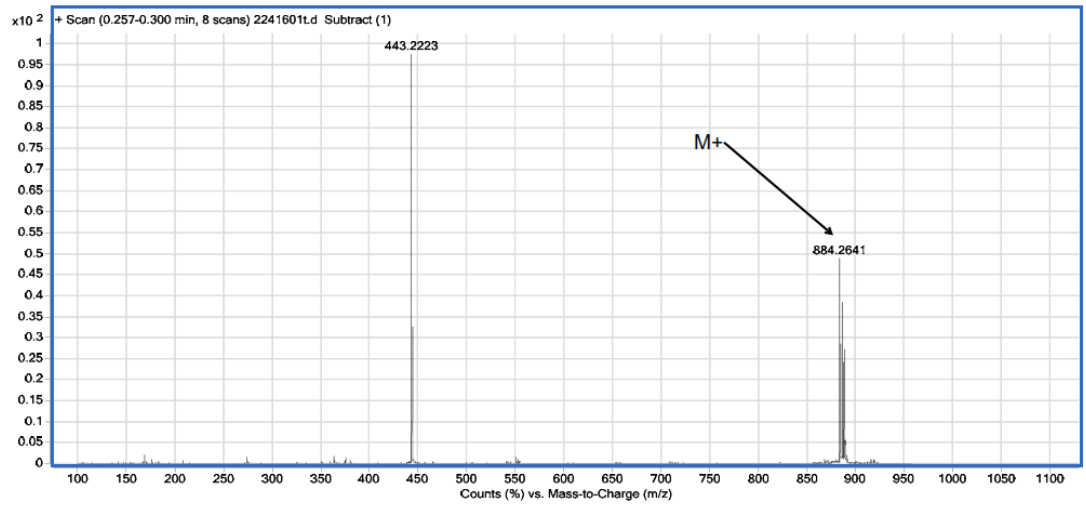
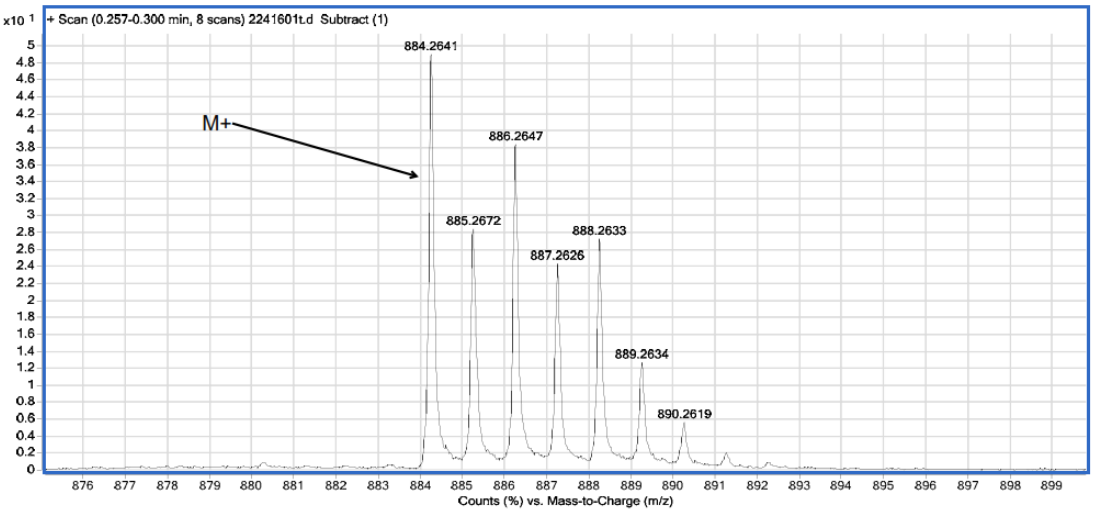


Figure S48. FT-IR of **16** in KBr.





Measured Mass 884.2641

Element	Low Limit	High Limit
C	47	57
H	35	55
N	3	7
O	0	5
S	0	1
Zn	0	1

Formula	Calculated Mass	mDaError	ppmError	RDB
C57 H46 N3 O S Zn	884.2648	-0.7	-0.7	36.5
C55 H44 N6 S Zn	884.2634	0.7	0.8	37
C53 H38 N7 O5 S	884.2650	-0.9	-1.0	38.5
C51 H44 N6 O5 Zn	884.2659	-1.8	-2.1	33
C52 H46 N5 O3 S Zn	884.2607	3.4	3.8	32.5

Figure S49. ESI/APCI MS of **16**.

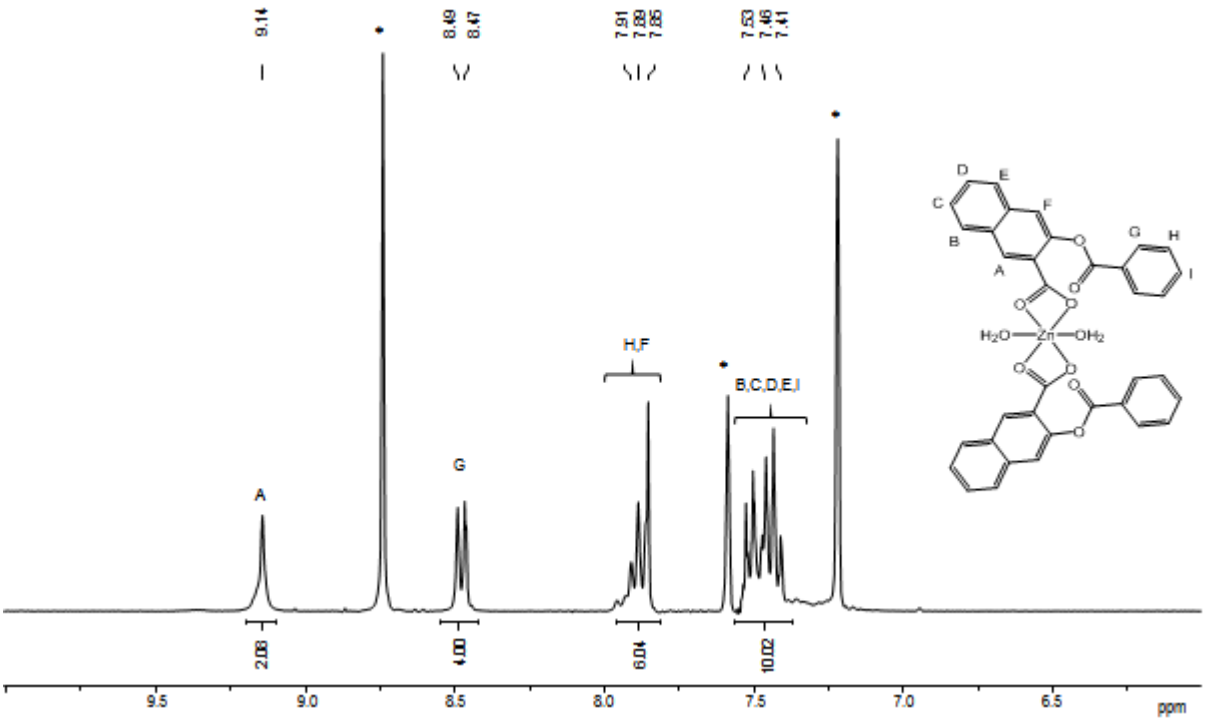


Figure S50. ^{1}H NMR spectrum of **17** in pyridine-d_5. (* denotes residual solvent peaks)

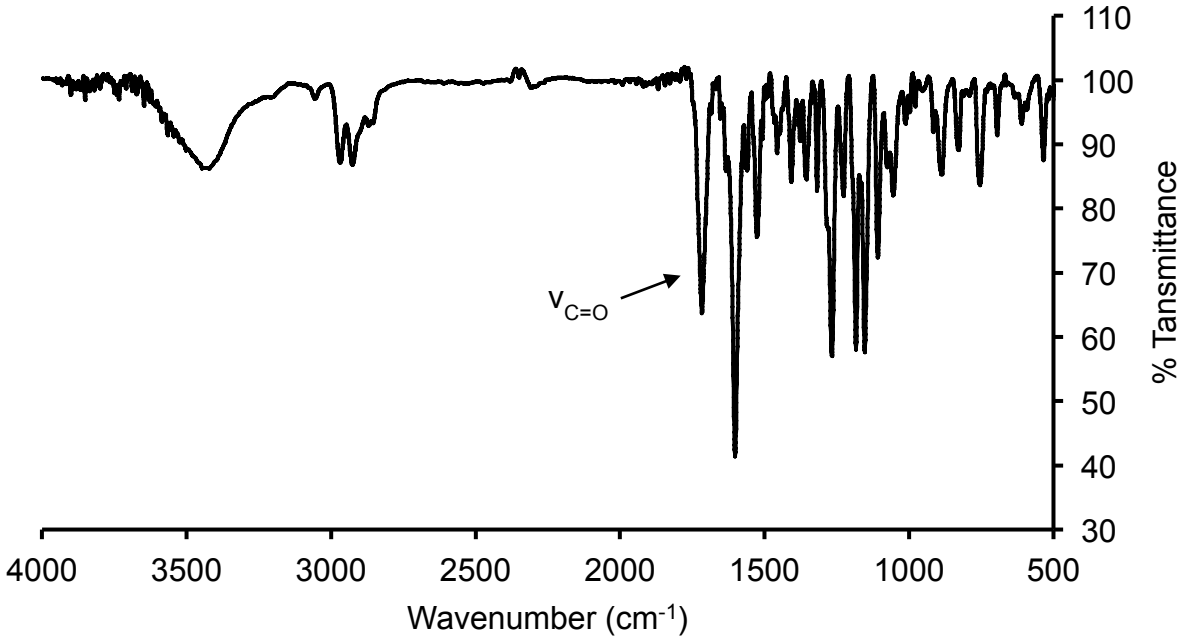


Figure S51. FT-IR spectrum of **17**.

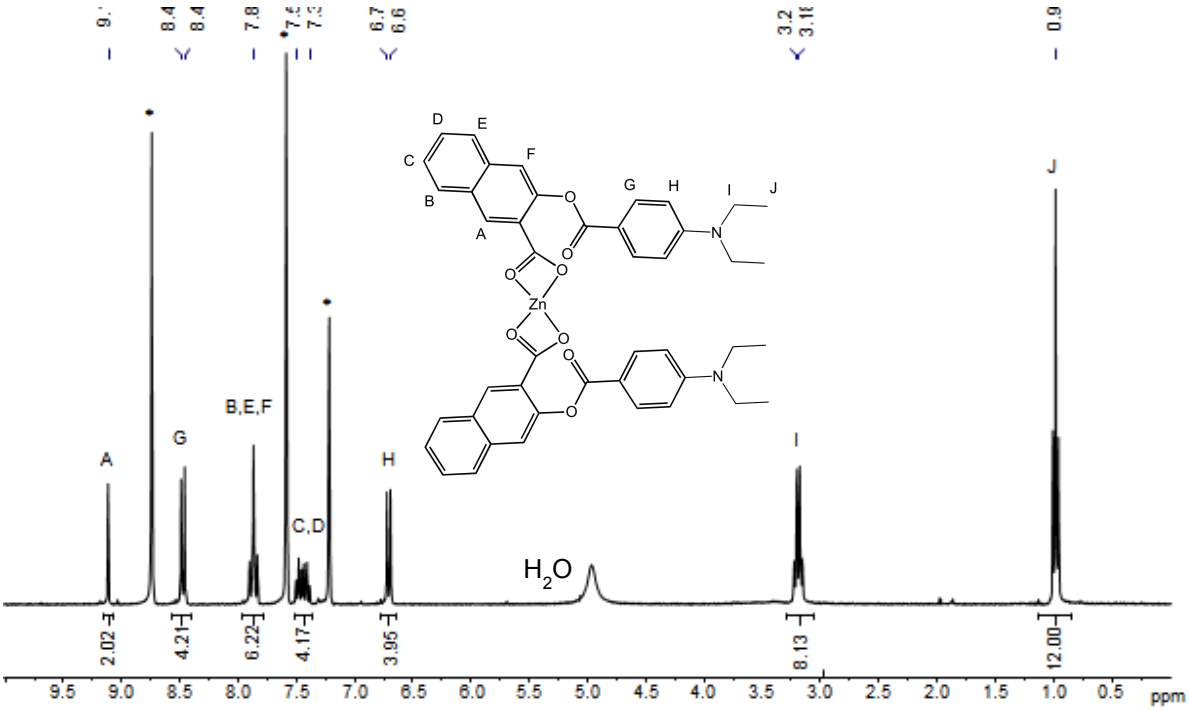


Figure S52. ^{1}H NMR spectrum of **18** in pyridine-d_5 (* denotes residual solvent peaks).

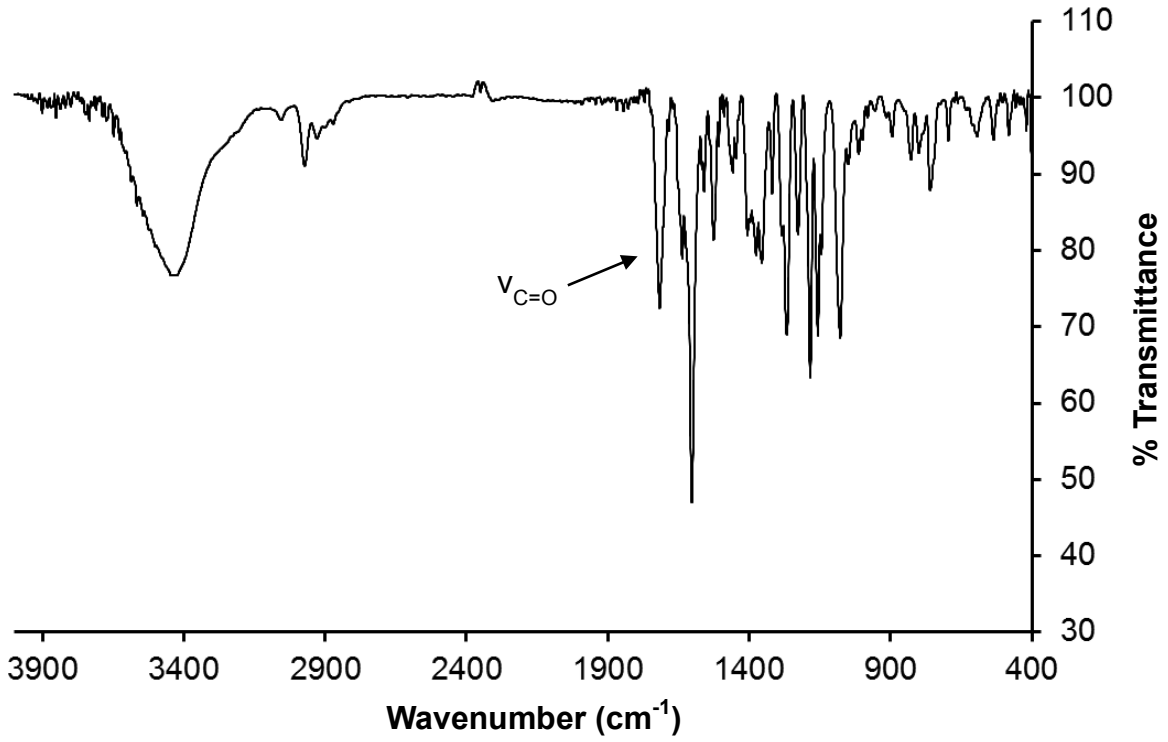


Figure S53. FT-IR spectrum of **18**.

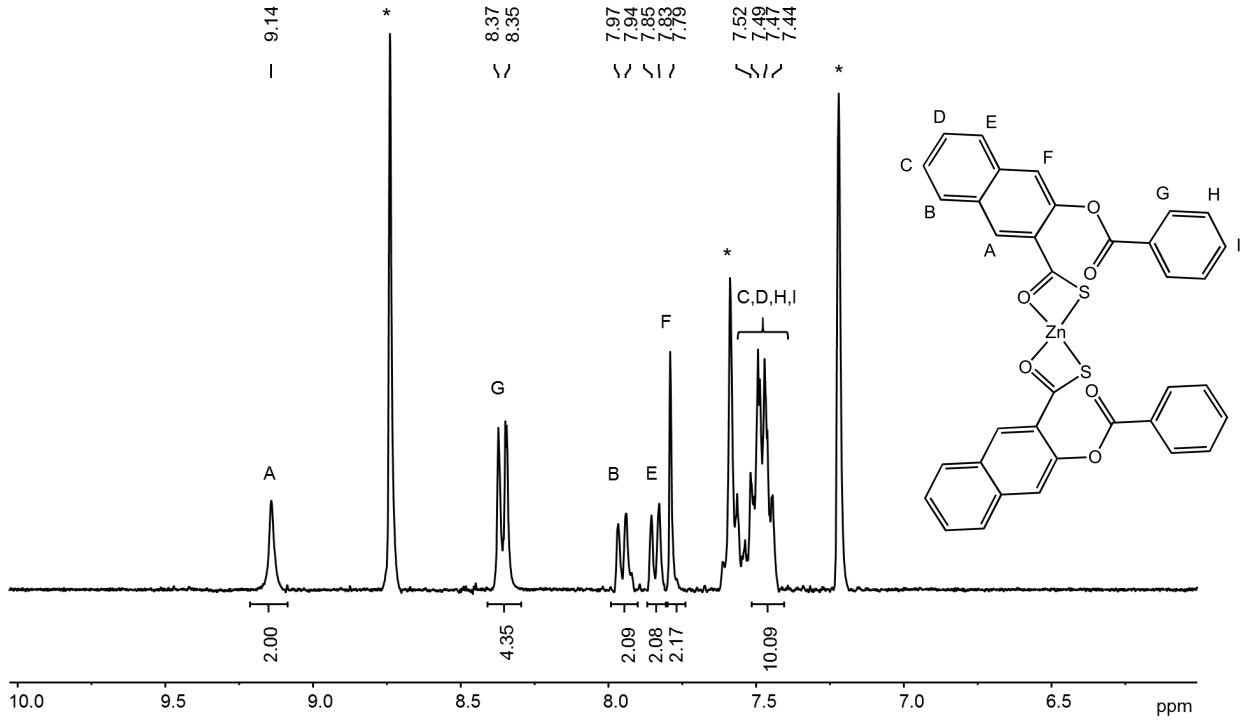


Figure S54. ^{1}H NMR spectrum of **19** in pyridine-d_5 (* denotes residual solvent).

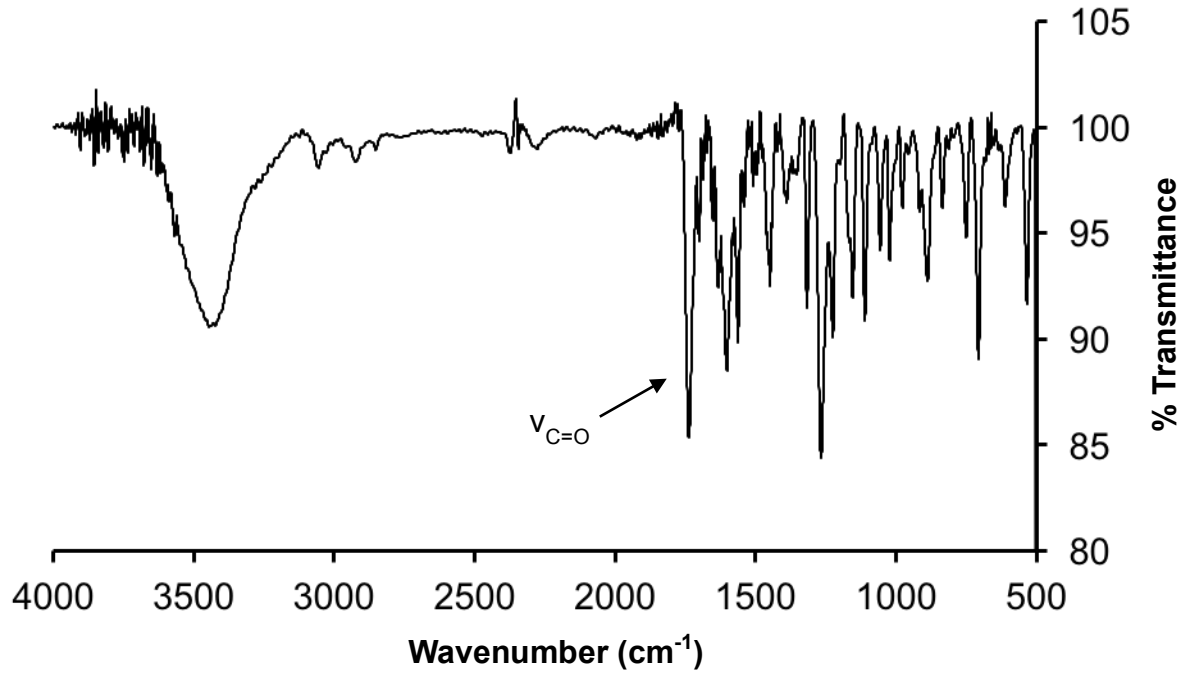


Figure S55. FT-IR spectrum of **19**.

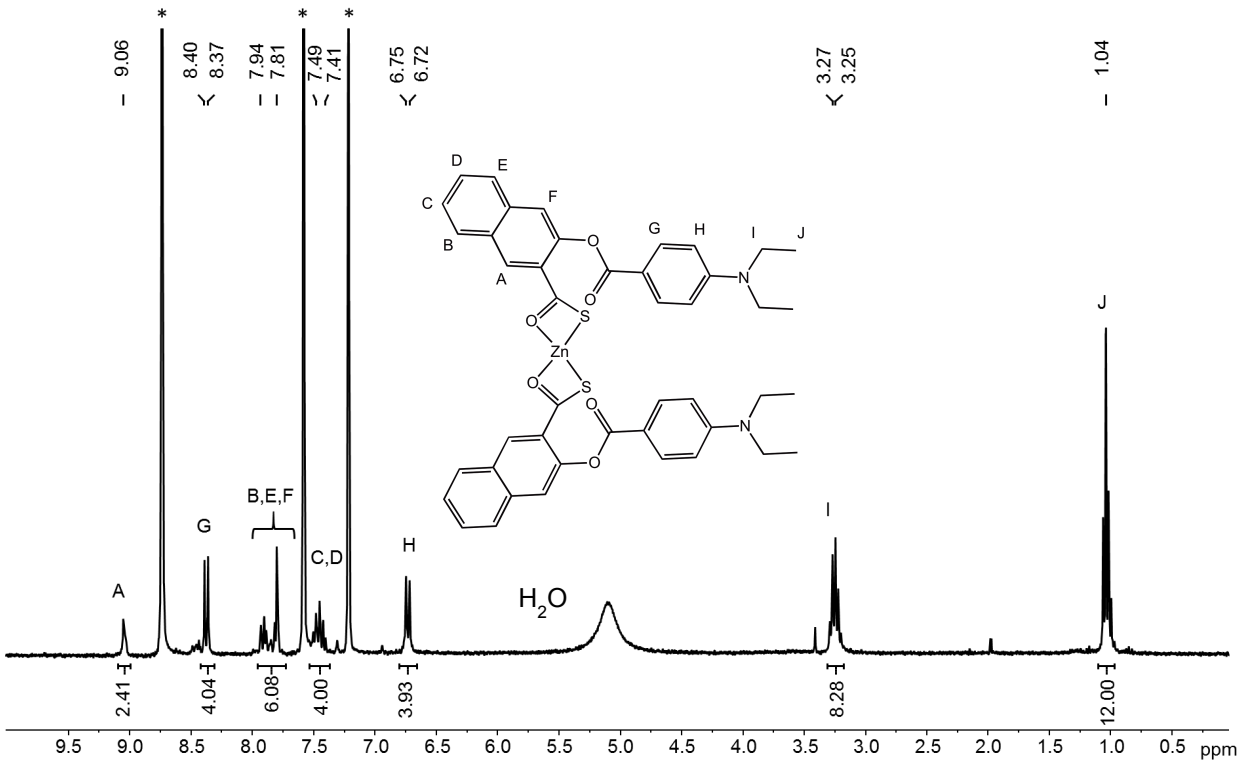


Figure S56. ^{1}H NMR spectrum of **20** in pyridine-d_5. (* denotes residual solvent)

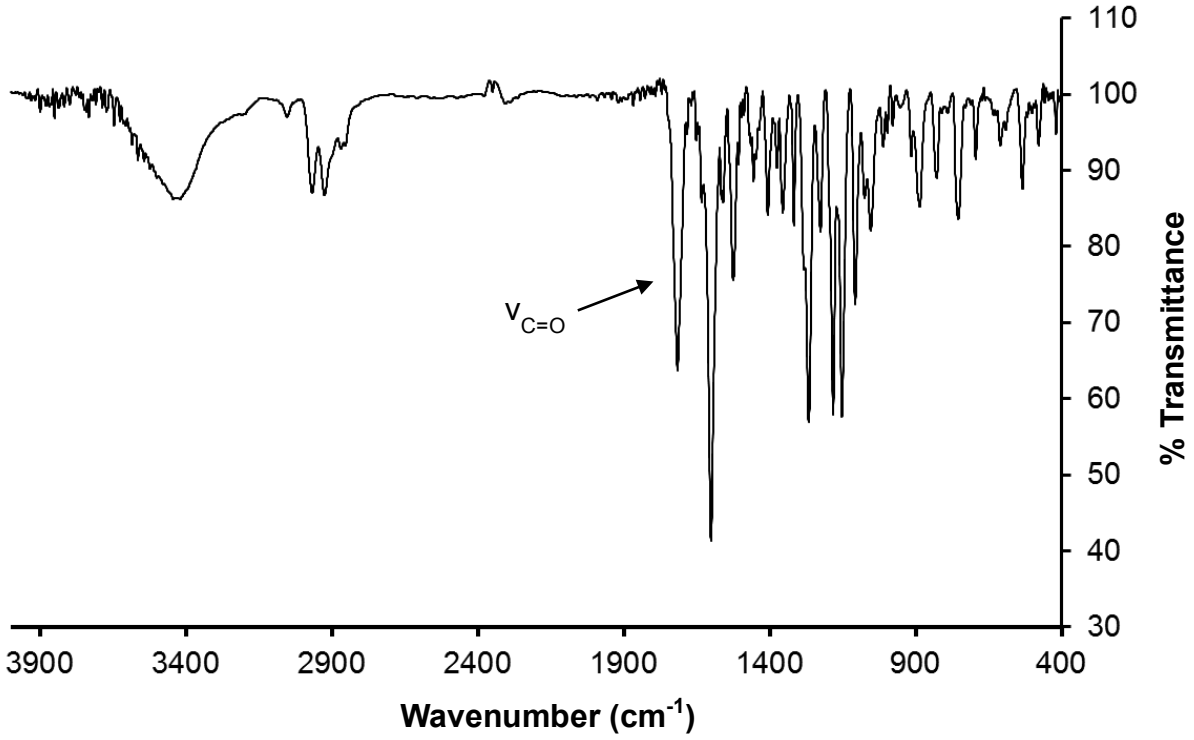


Figure S57. FT-IR spectrum of **20**.

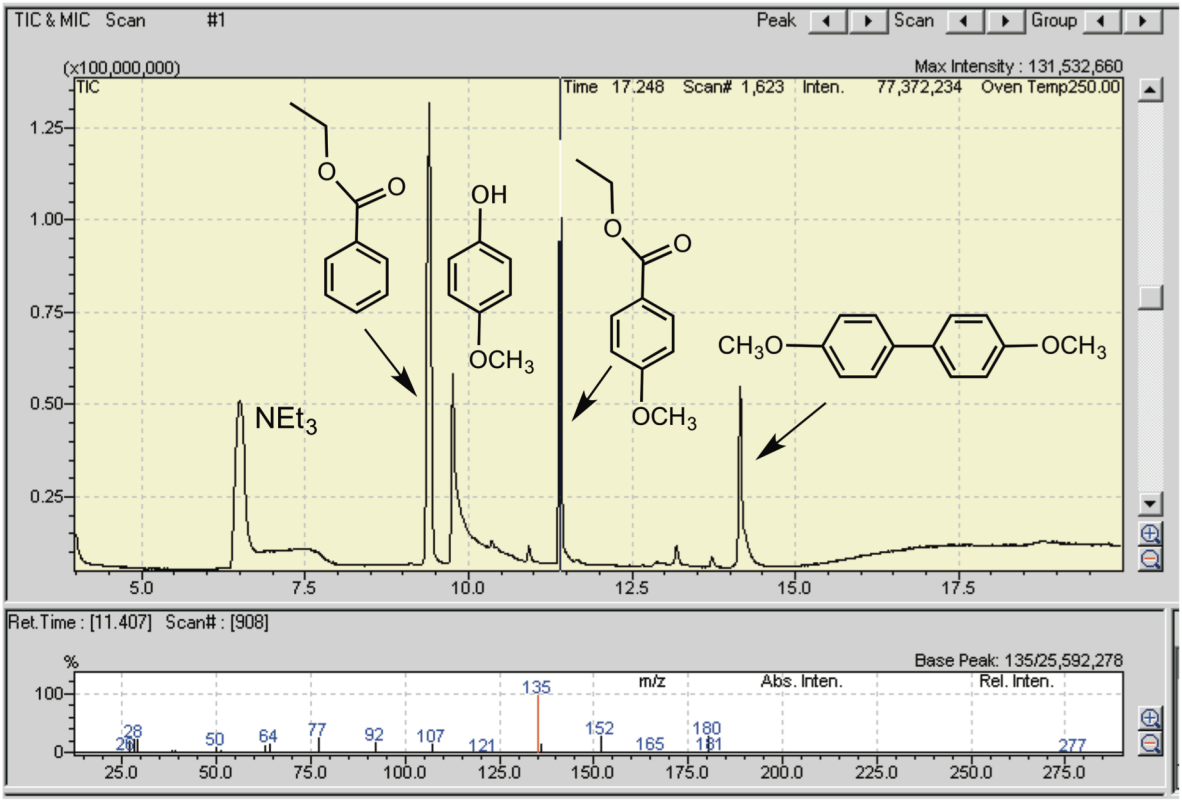


Figure S58. GC-MS results for the carbonylation reaction of **21a** using a film of **9** as the light-induced CO source.

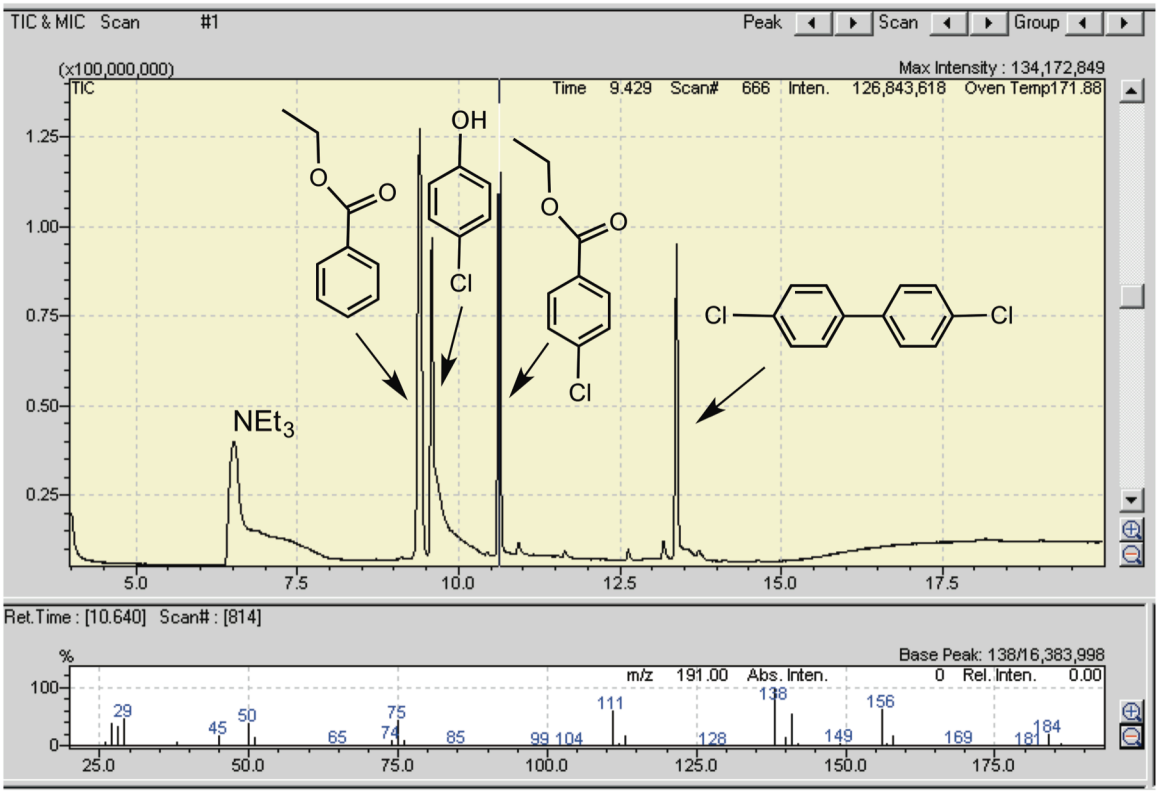


Figure S59. GC-MS results for the carbonylation reaction of **21b** using a film of **9** as the light-induced CO source.

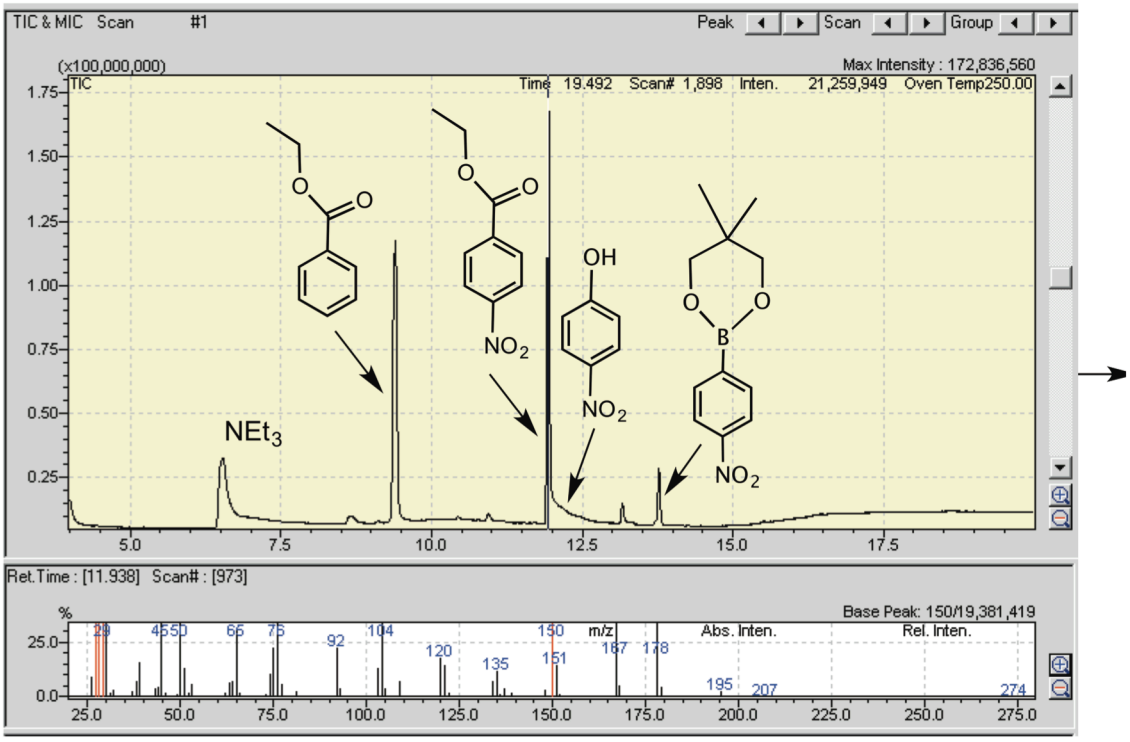


Figure S60. GC-MS results for the carbonylation reaction of **21c** using a film of **9** as the light-induced CO source.

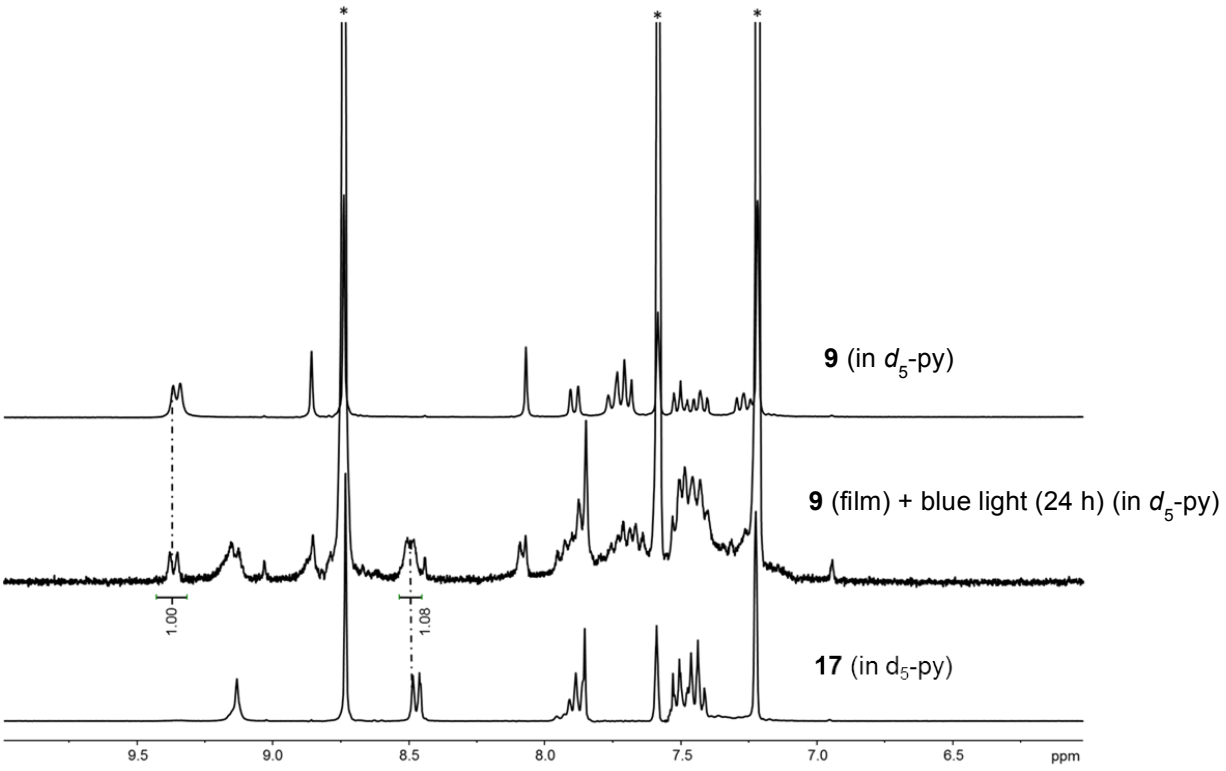


Figure S61. ^{1}H NMR spectrum of **9** in pyridine-d_5 (top). ^{1}H NMR spectrum of remaining solid following illumination of **9** (film) with two blue CFL bulbs for 24 hours (middle). ^{1}H NMR spectrum of **17** in pyridine-d_5 (bottom) (* denotes residual solvent).