Supporting Information
For

Competitive Electronic Effect of Ligand's Substitution over the Role of Metal Ions (Ni and Co) on Unusual Amine-Imine Inter-conversion in Conjugated Amine-ene-imine Ligands

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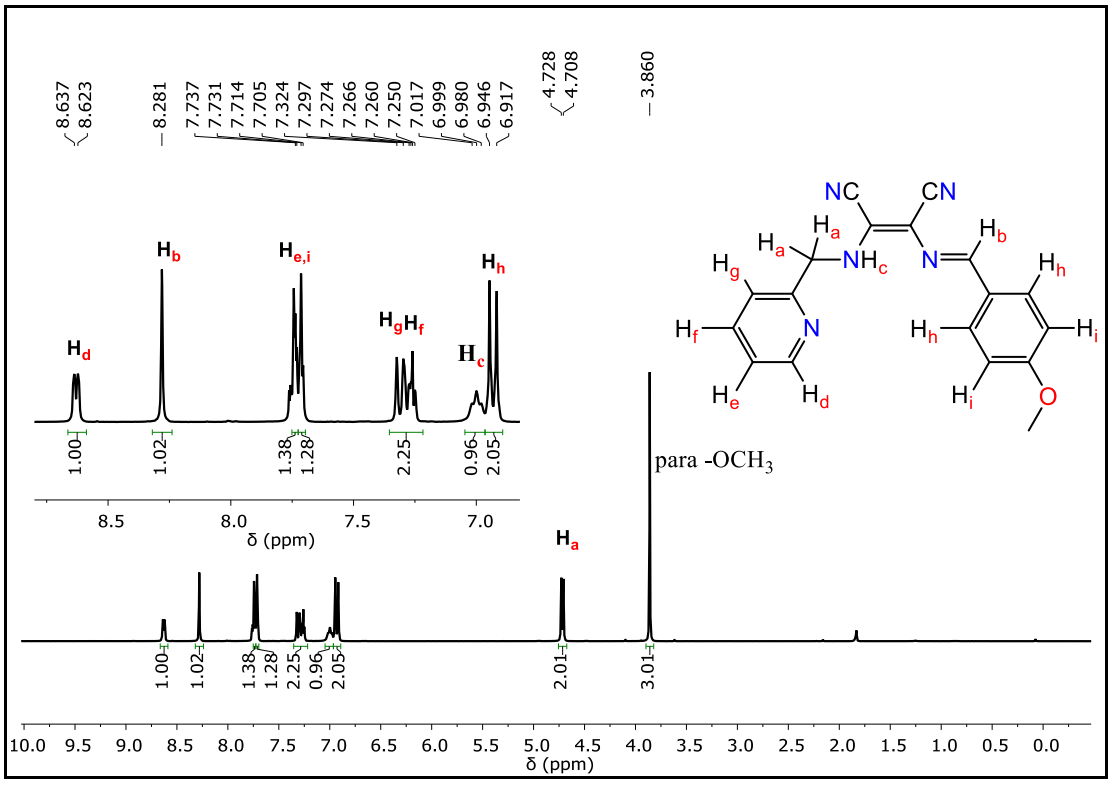


Figure S1: ^{1}H NMR Spectrum of $HL^{1\text{-}OMe}$ in $CDCl_3$.

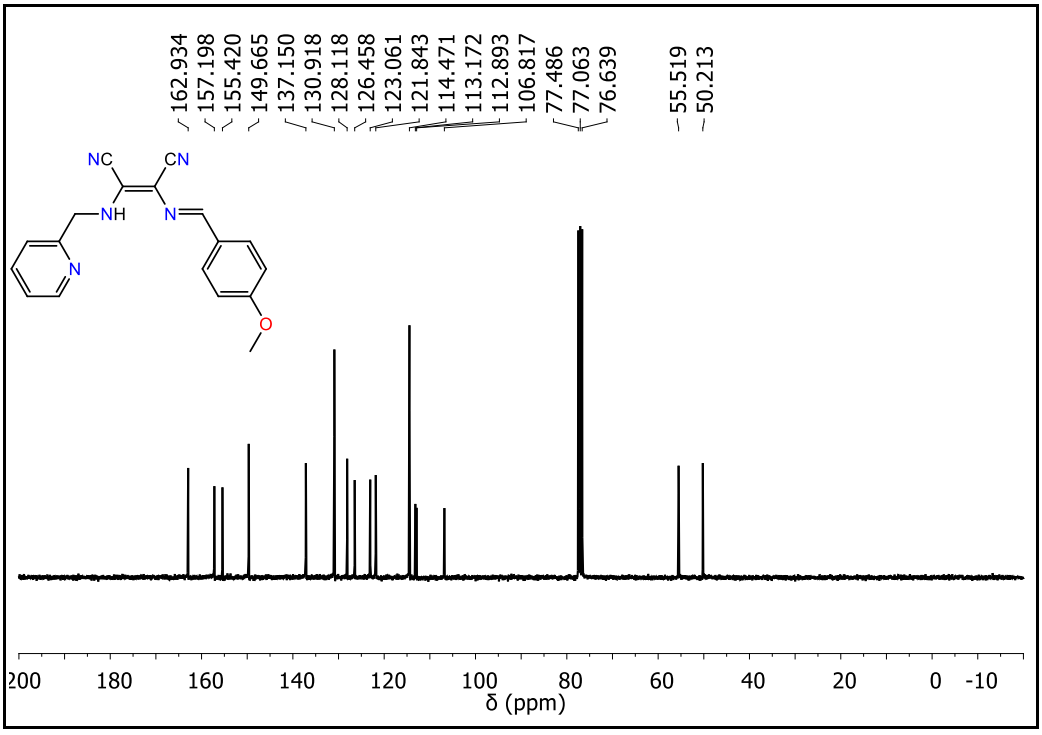


Figure S2: ^{13}C NMR Spectrum of $HL^{1\text{-}OMe}$ in CDC

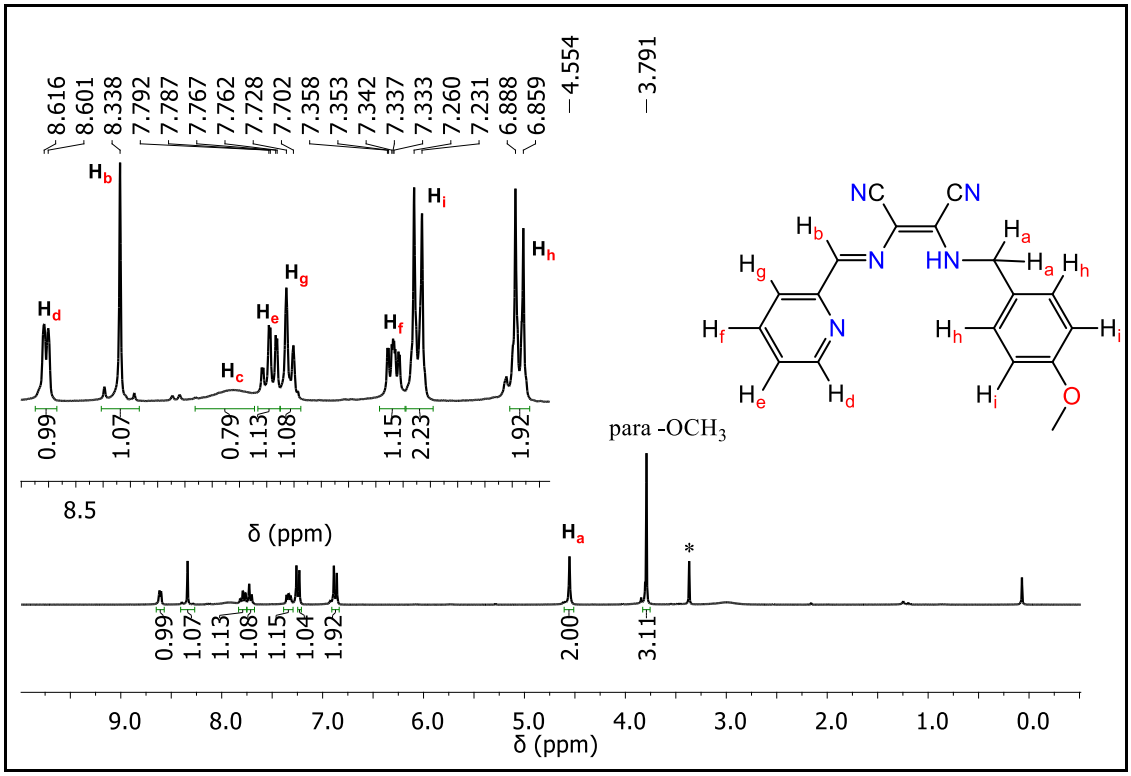


Figure S3: ^{1}H NMR Spectrum of **HL$^{2\text{-OMe}}$** in $CDCl_3$.

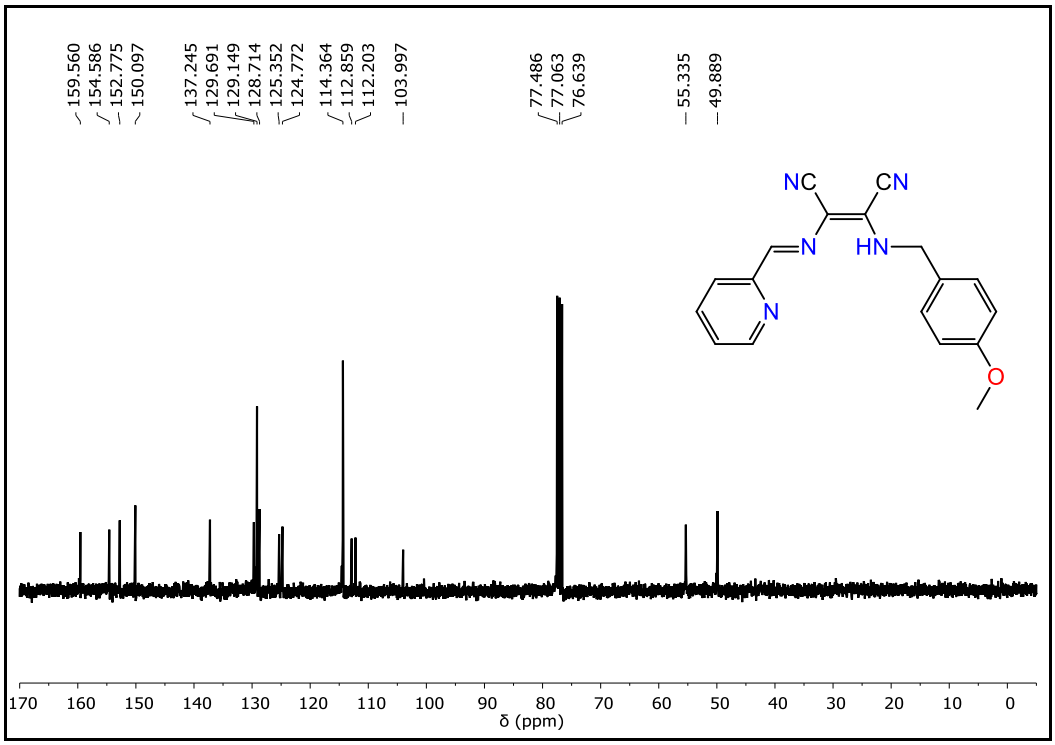


Figure S4: ^{13}C NMR Spectrum of **HL$^{2\text{-OMe}}$** in $CDCl_3$.

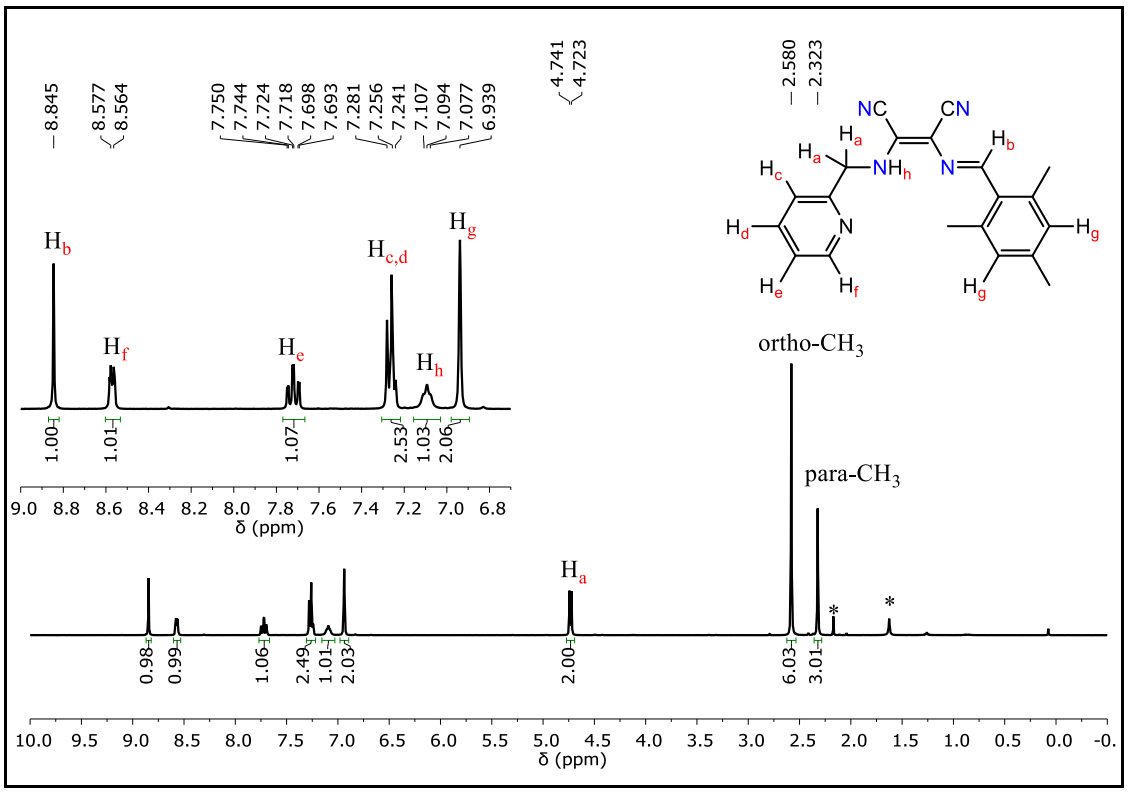


Figure S5: ^{1}H NMR Spectrum of **HL**$^{1\text{-Mes}}$ in $CDCl_3$.

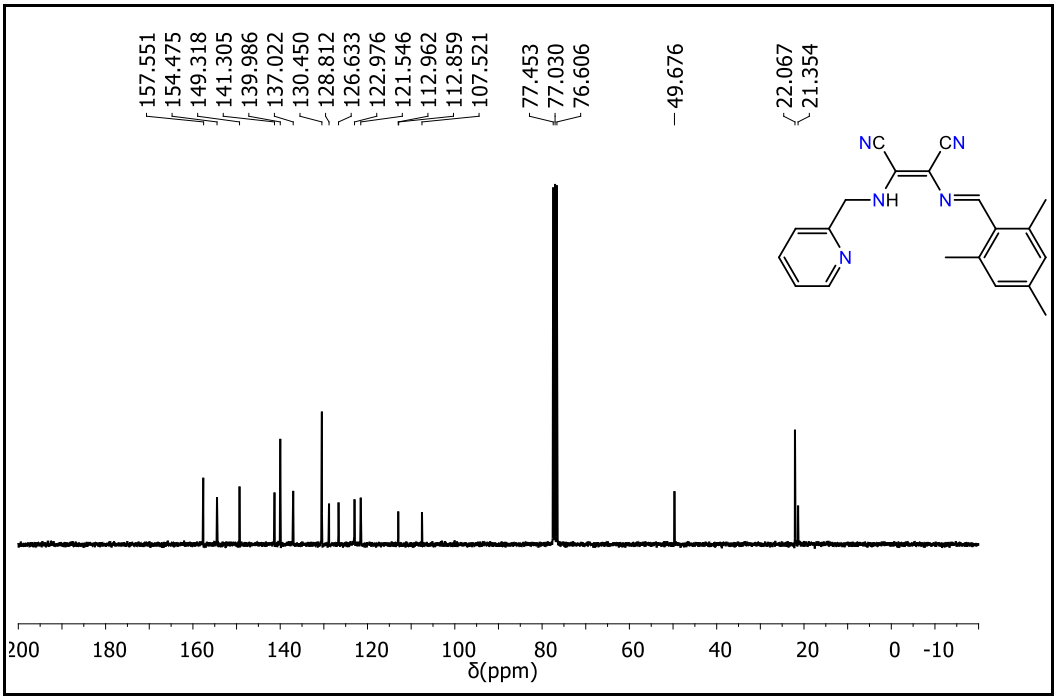


Figure S6: ^{13}C NMR Spectrum of **HL**$^{1\text{-Mes}}$ in $CDCl_3$.

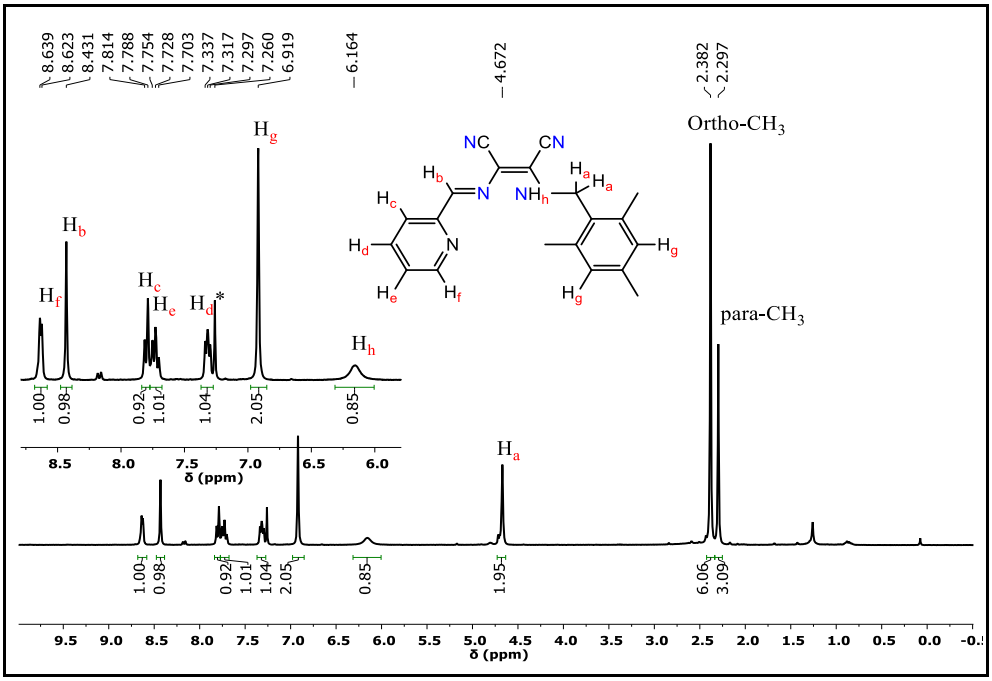


Figure S7: ^{1}H NMR Spectrum of **HL**$^{\mathbf{2\text{-}Mes}}$ in $CDCl_3$.

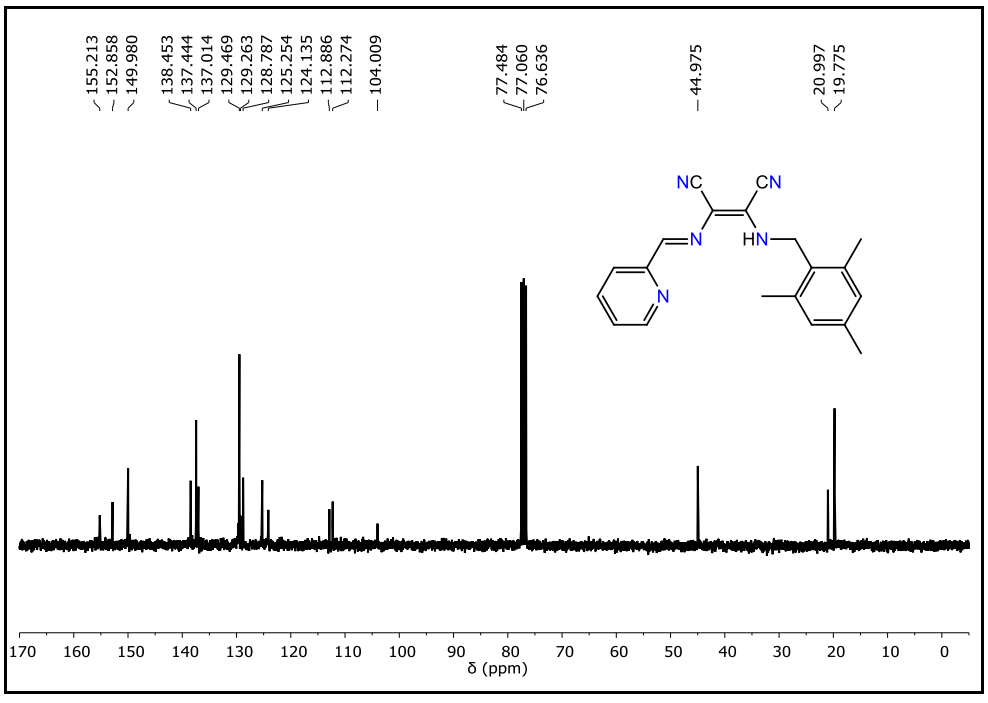


Figure S8: ^{13}C NMR Spectrum of **HL**$^{\mathbf{2\text{-}Mes}}$ in $CDCl_3$.

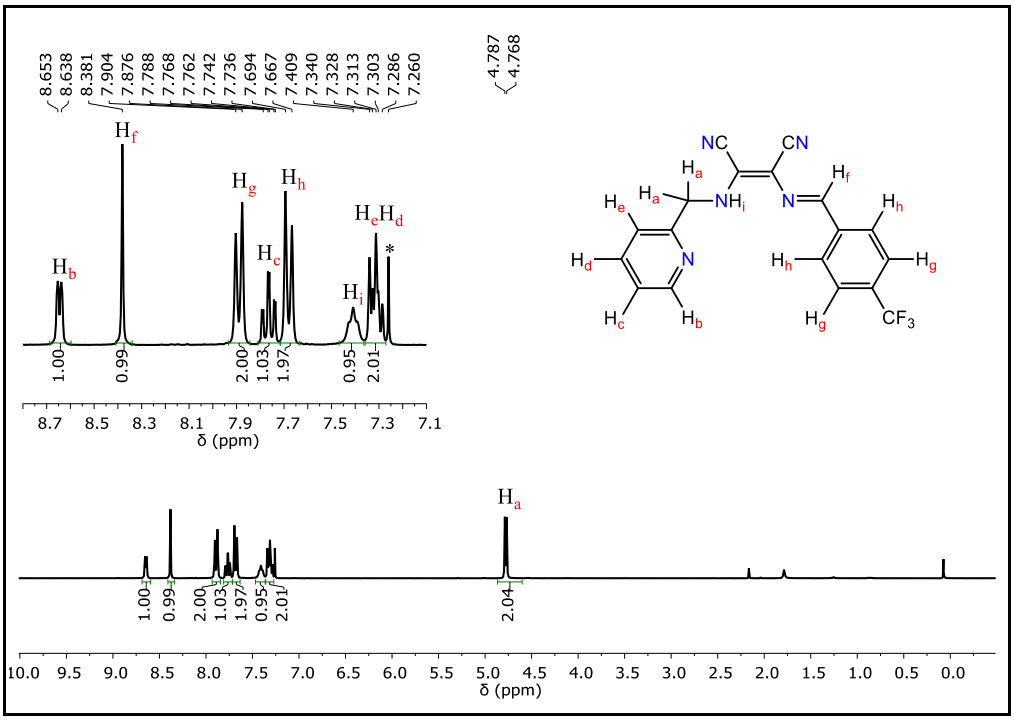


Figure S9: ^{1}H NMR Spectrum of **HL$^{1\text{-}CF3}$** in $CDCl_3$.

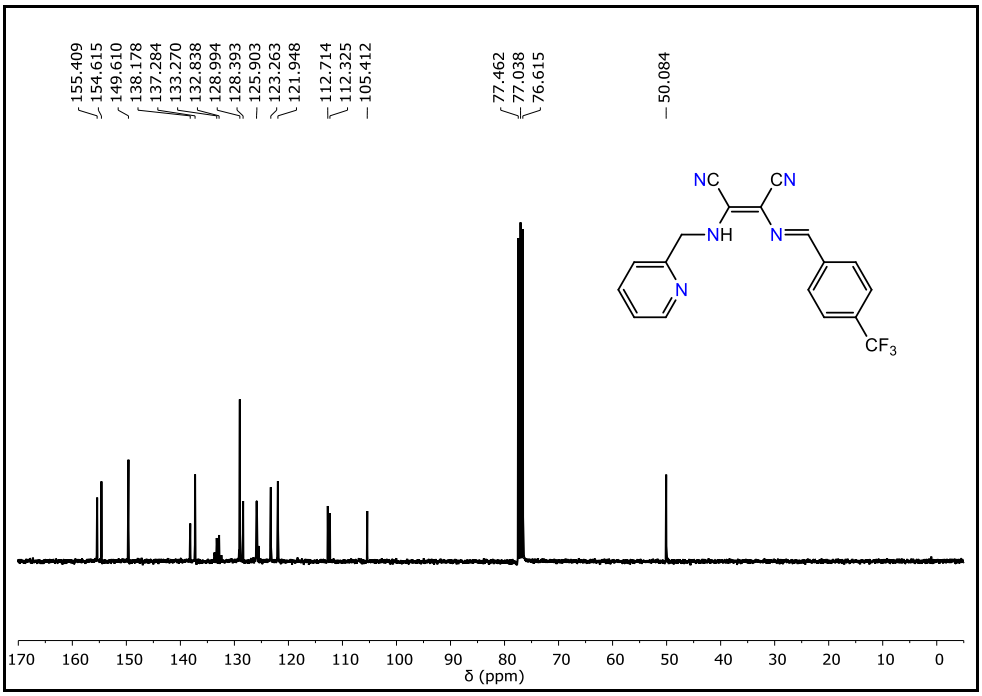


Figure S10: ^{13}C NMR Spectrum of **HL$^{1\text{-}CF3}$** in $CDCl_3$.

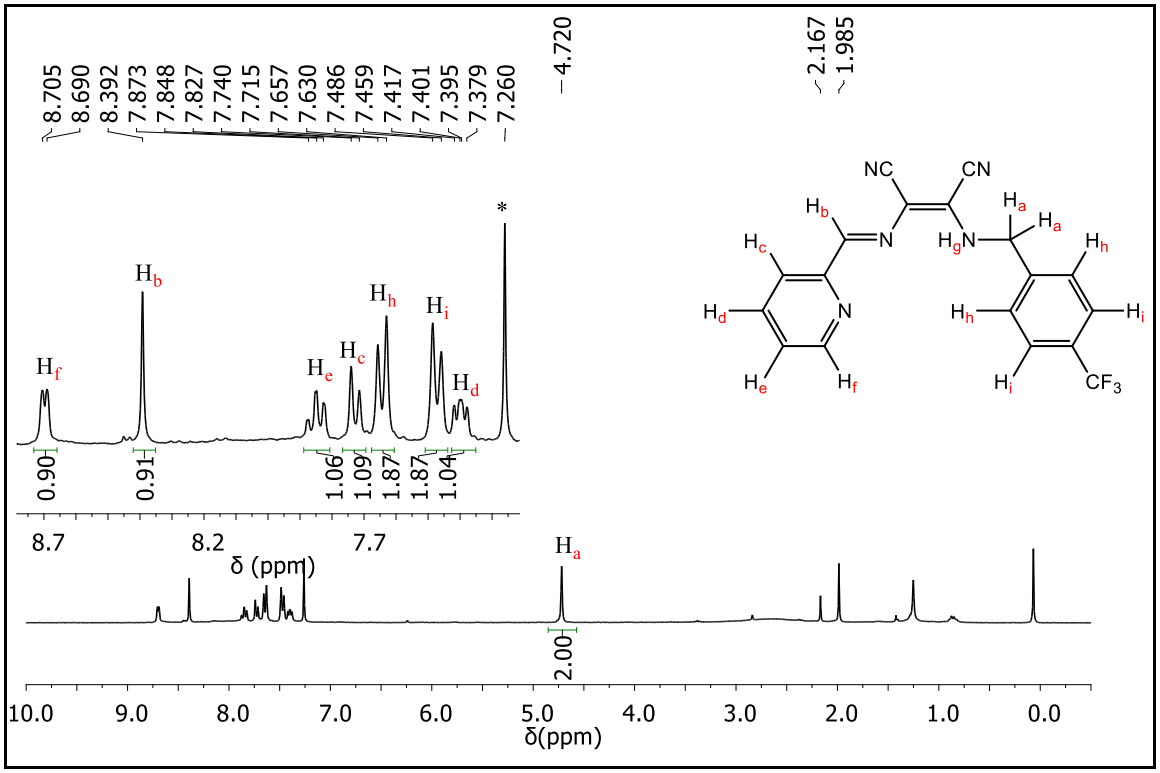


Figure S11: ^{1}H NMR Spectrum of HL$^{2\text{-}CF3}$ in $CDCl_3$.

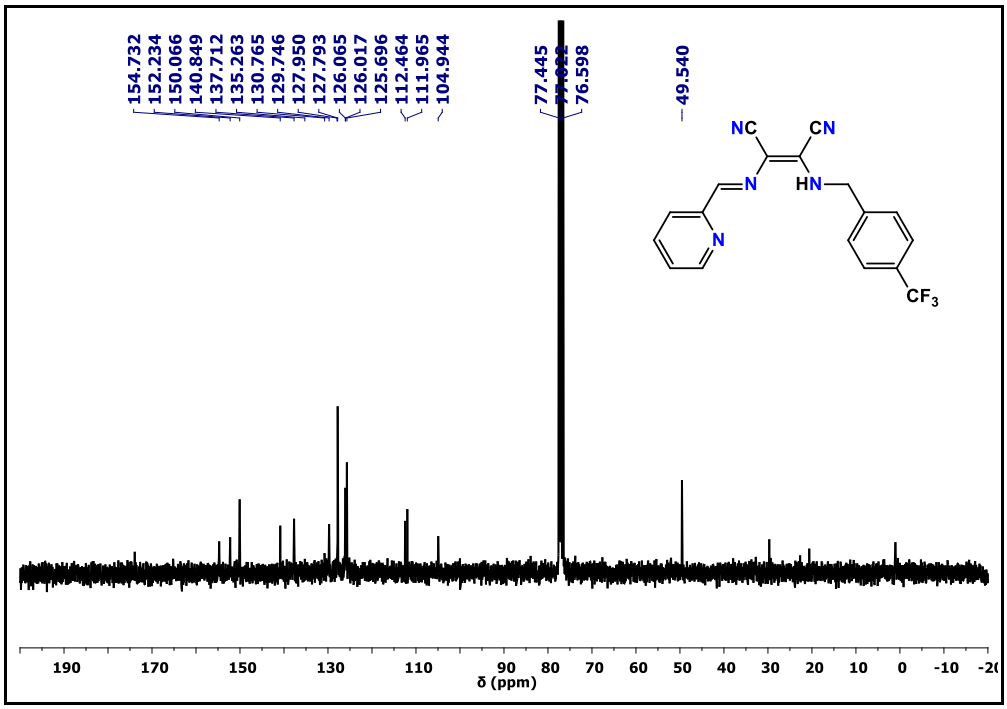


Figure S12: ^{13}C NMR Spectrum of **HL$^{2\text{-}CF3}$ in $CDCl_3$.**

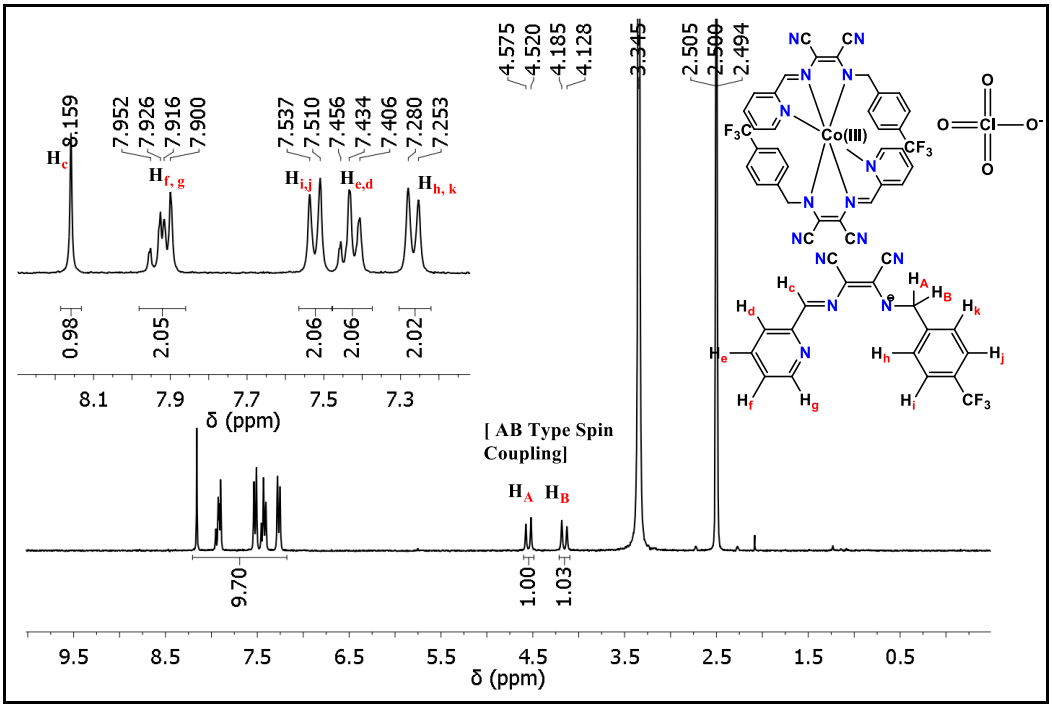


Figure S13: ^{1}H NMR Spectrum of **Co$^{2\text{-}CF3}$.ClO$_4$** in d$_6$-DMSO.

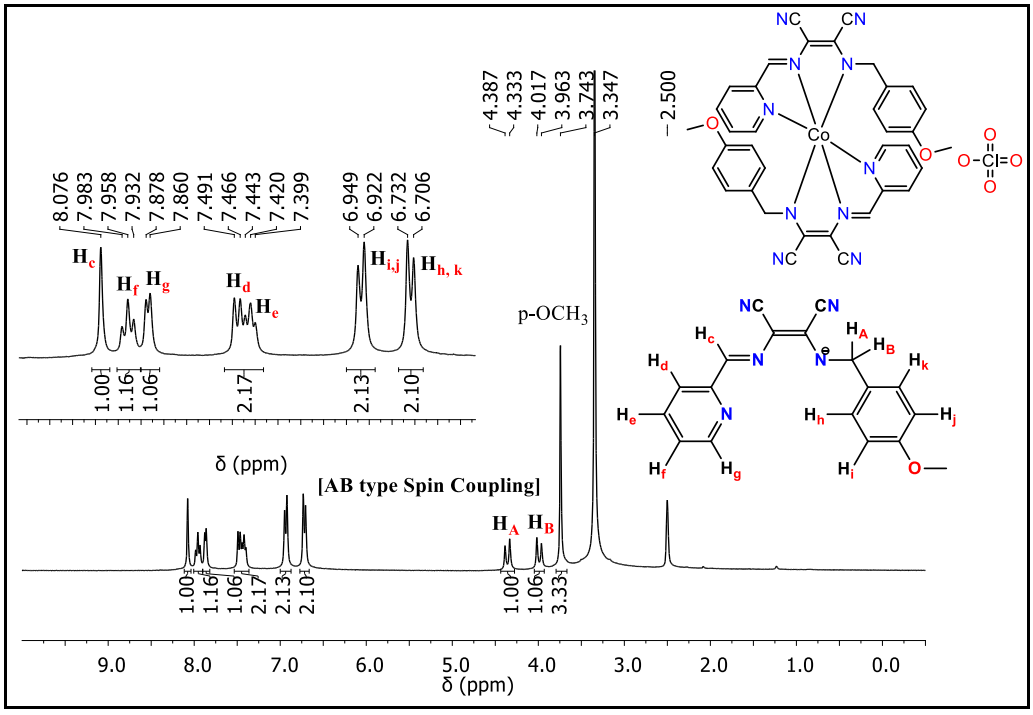


Figure S14: ^{1}H NMR Spectrum of **Co$^{2\text{-}OMe}$.ClO$_4$** in d$_6$-DMSO.

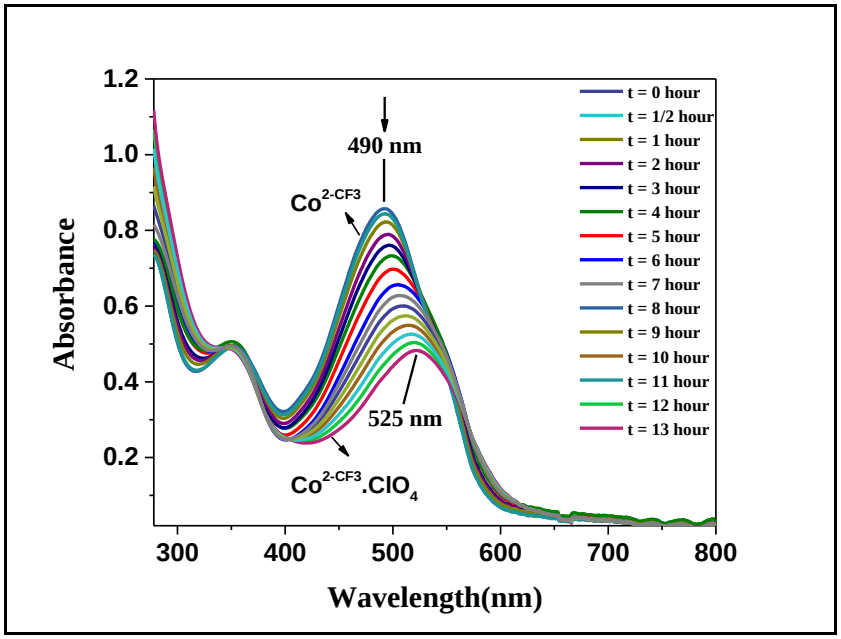


Figure S15: Electronic absorption spectral changes for arial oxidation of $\mathbf{Co^{2\text{-}CF3}}$(obtained from bulk electrolysis) to $\mathbf{Co^{2\text{-}CF3}.ClO_4(0.5 \times 10^{-4}\ M)}$ in acetonitrile.

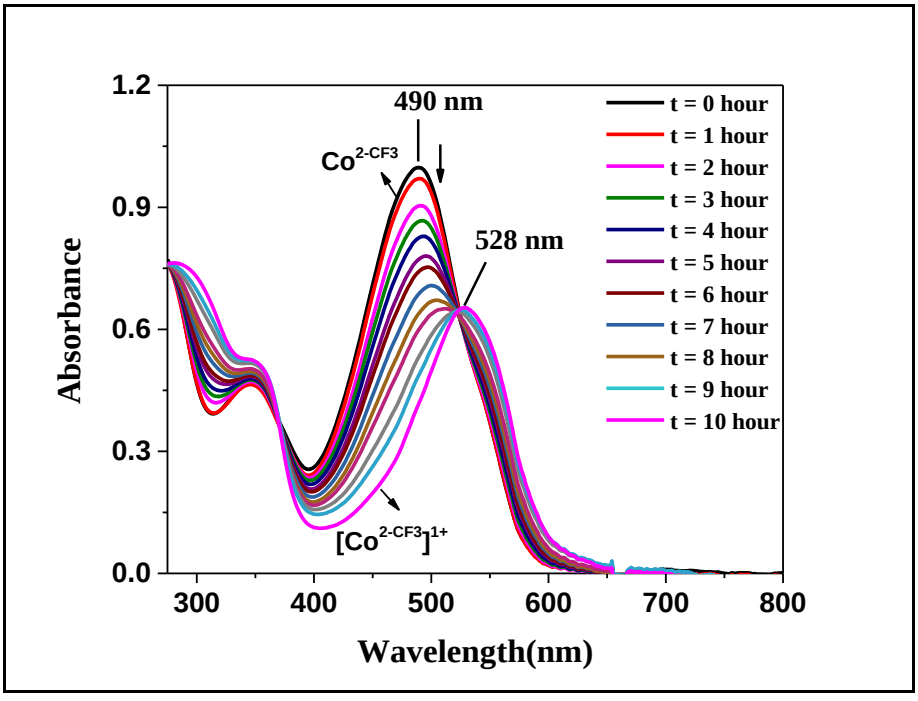


Figure S16: Electronic absorption spectral changes for arial oxidation of $\mathbf{Co^{2\text{-}CF3}}$ (isolated from the reaction of **Co(II)** and $\mathbf{H_2L^{2\text{-}CF3}}$) to $\mathbf{[Co^{2\text{-}CF3}]^{1+}}$ (0.5×10^{-4} M) in acetonitrile.

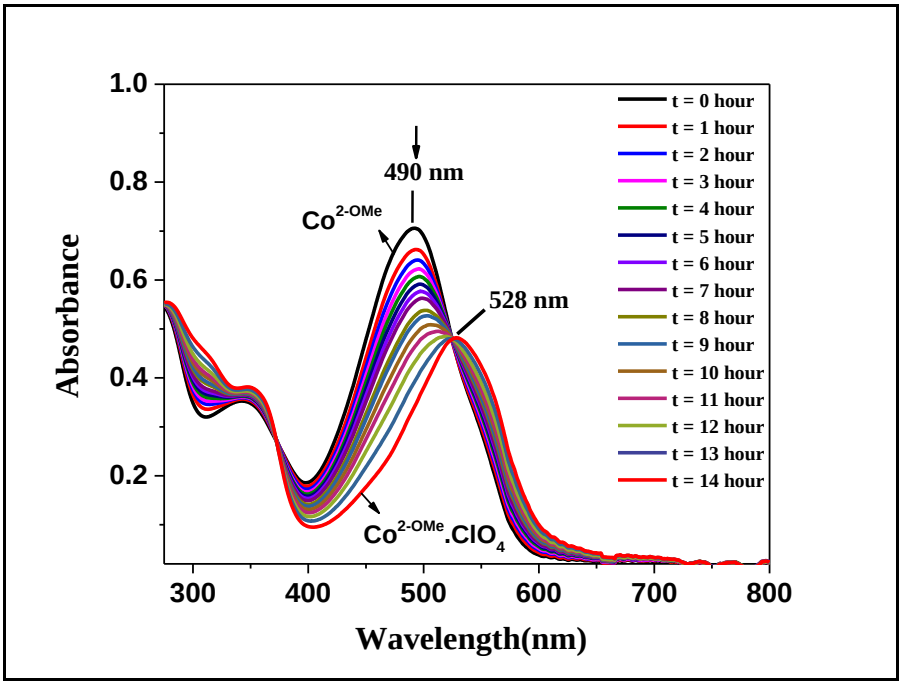


Figure S17: Electronic absorption spectral changes for arial oxidation of $\mathbf{Co^{2\text{-}OMe}}$(obtained from bulk electrolysis) to $\mathbf{Co^{2\text{-}OMe}.ClO_4}$ (0.5 x 10^{-4} M) in acetonitrile.

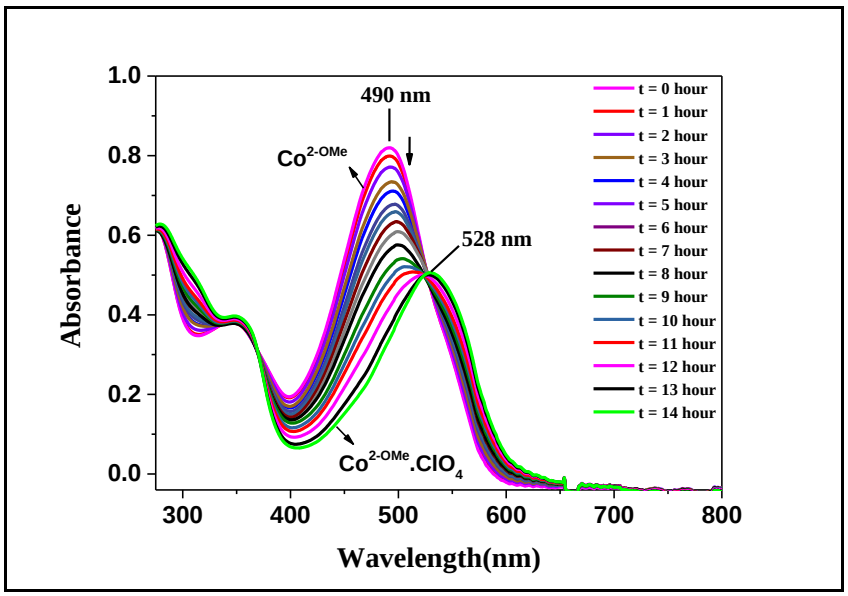


Figure S18: Electronic absorption spectral changes for arial oxidation of $\mathbf{Co^{2\text{-}OMe}}$ (isolated from the reaction of **Co(II) and** $\mathbf{H_2L^{2\text{-}OMe}}$**)** to $\mathbf{[Co^{2\text{-}OMe}]^{1+}}$ (0.5 x 10^{-4} M) in acetonitrile.

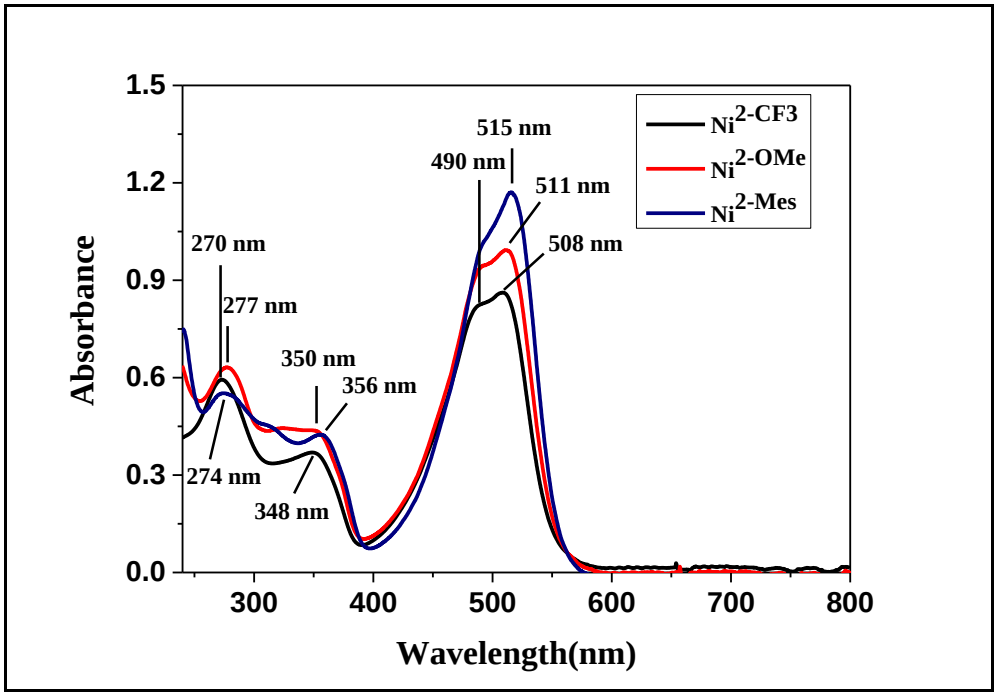


Figure S19: Electronic absorption spectra of **Ni$^{2\text{-}CF3}$**, **Ni$^{2\text{-}OMe}$** and **Ni$^{2\text{-}Mes}$**, (2.5 x 10^{-5} M) in acetonitrile.

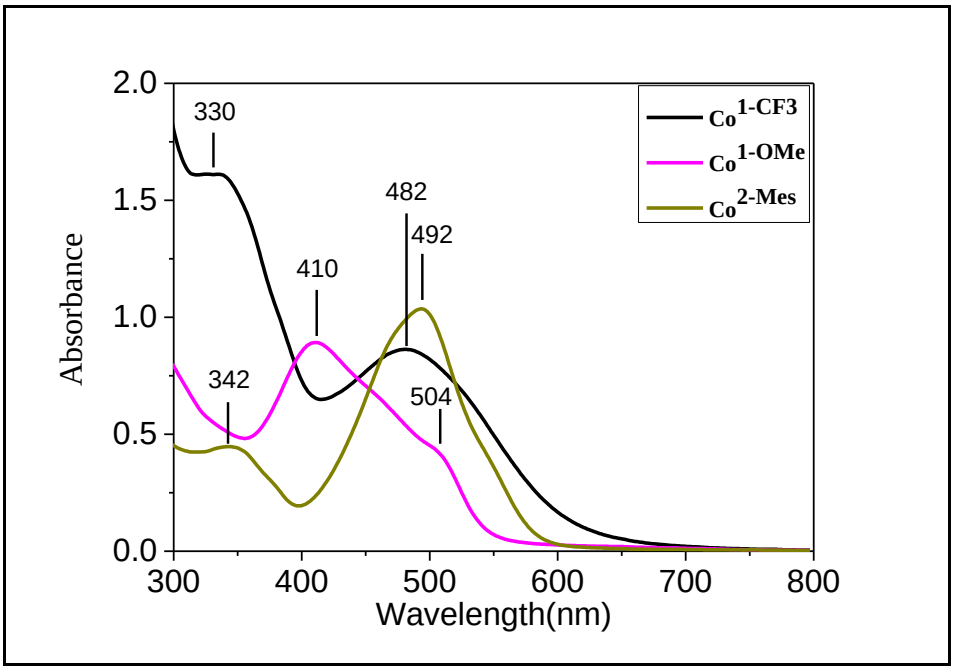


Figure S20: Electronic absorption spectra of **Co$^{1\text{-}CF3}$**, **Co$^{1\text{-}OMe}$** and **Co$^{2\text{-}Mes}$** (0.5 x 10^{-4} M) in acetonitrile.

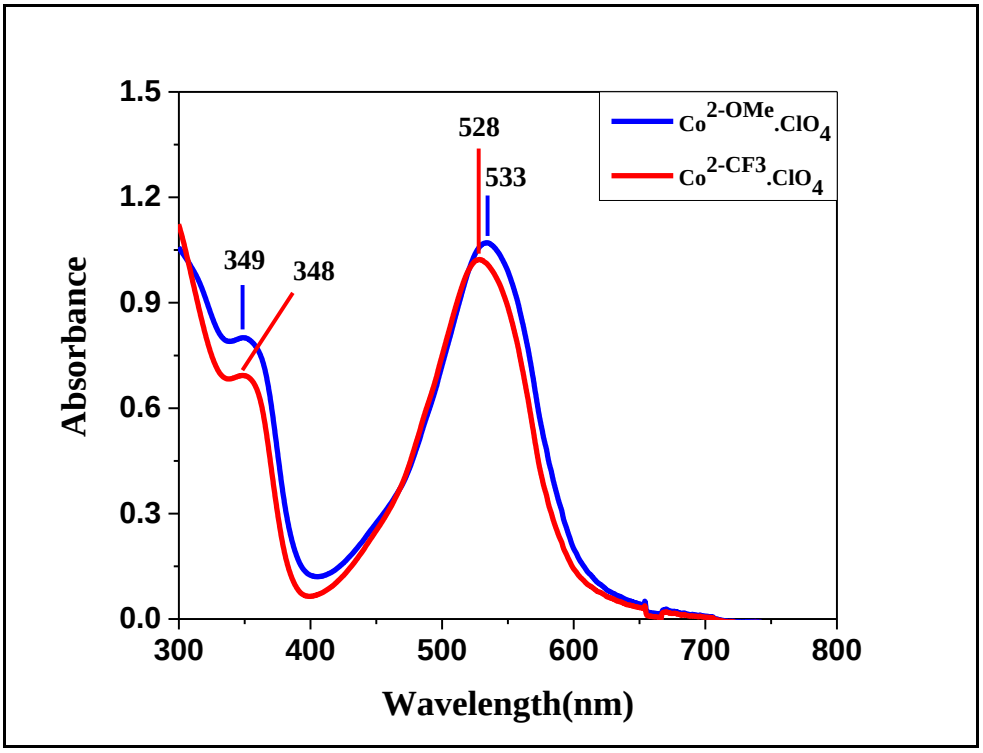


Figure S21: Electronic absorption spectra of $\mathbf{Co^{2\text{-}CF3}ClO_4}$, $\mathbf{Co^{2\text{-}OMe}ClO_4}$ (10^{-4} M) in acetonitrile.

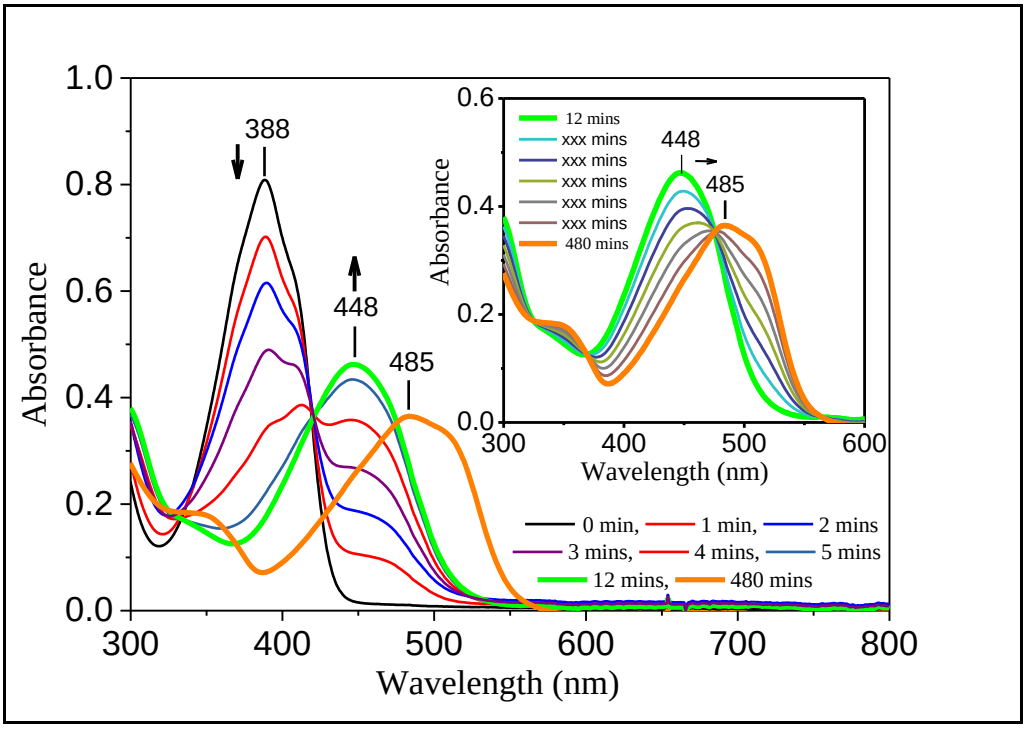


Figure S22: Electronic absorption spectral changes with time for the reaction of $Ni(ClO_4)_2.6H_2O$ (7.16×10^{-6}(M)) and $\mathbf{HL^{1\text{-}OMe}}$ (1.43×10^{-5}(M)) in acetonitrile to the formation of $\mathbf{Ni^{2\text{-}OMe}}$.

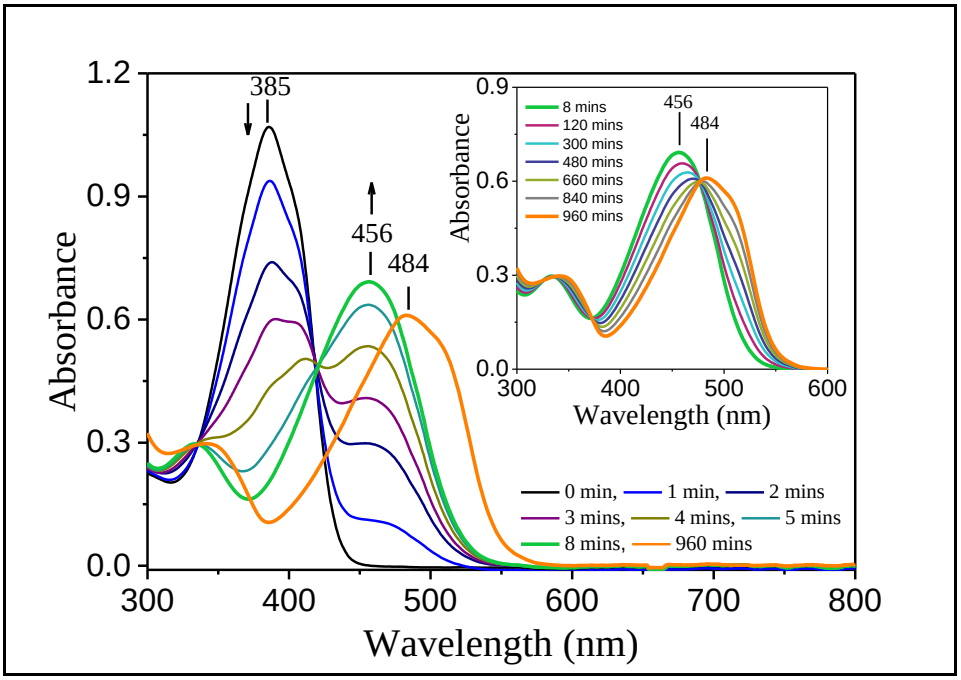


Figure S23: Electronic absorption spectral changes with time for the reaction of $Ni(ClO_4)_2.6H_2O$ (1.05×10^{-5}(M)) and **HL**$^{\mathbf{1\text{-}CF3}}$ (2.1×10^{-5} (M)) in acetonitrile to the formation of **Ni**$^{\mathbf{2\text{-}CF3}}$.

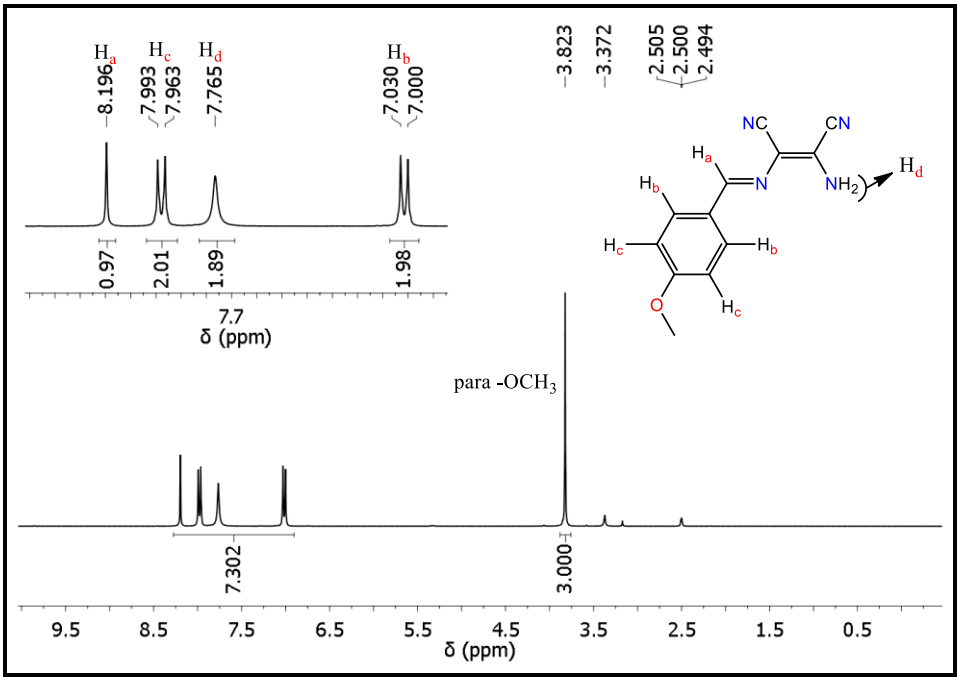


Figure S24: ^{1}H NMR Spectrum of **C**$^{\mathbf{OMe}}$ in d_6-DMSO

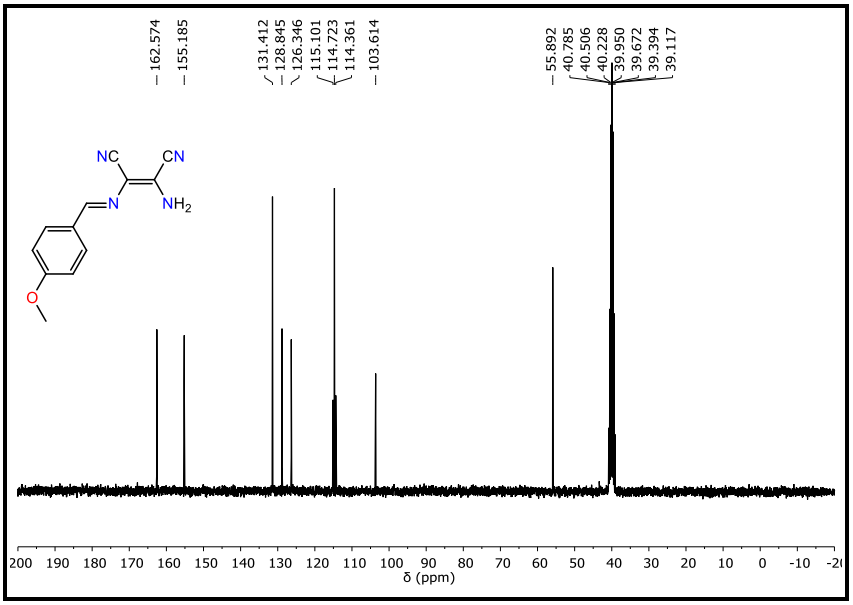


Figure S25: ^{13}C NMR Spectrum of $\mathbf{C}^{\mathbf{OMe}}$ in d_6-DMSO

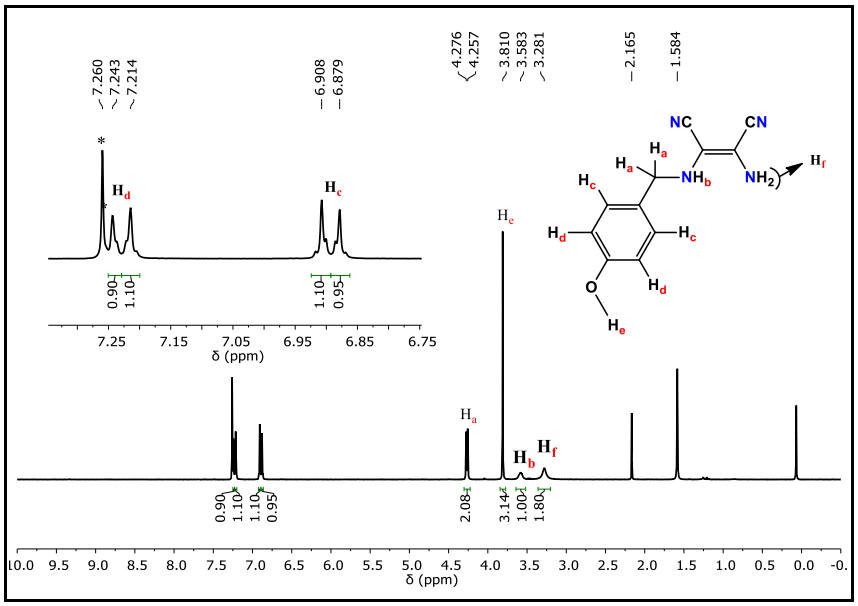


Figure S26: ^{1}H NMR Spectrum of $\mathbf{D}^{\mathbf{OMe}}$ in $CDCl_3$.

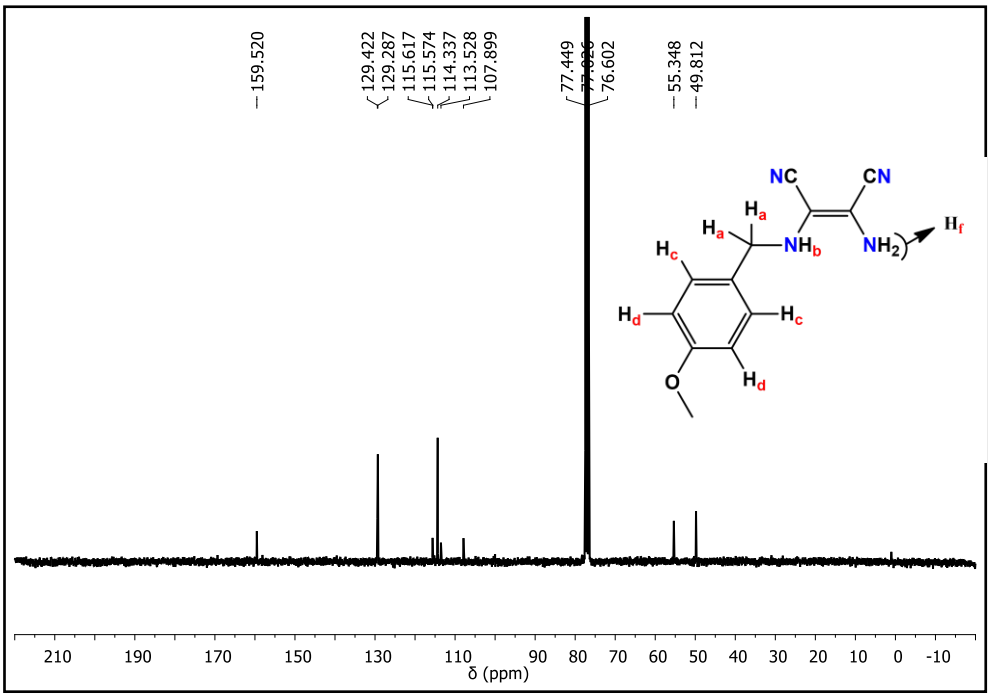


Figure S27: ^{13}C NMR Spectrum of $\mathbf{D^{OMe}}$ in $CDCl_3$

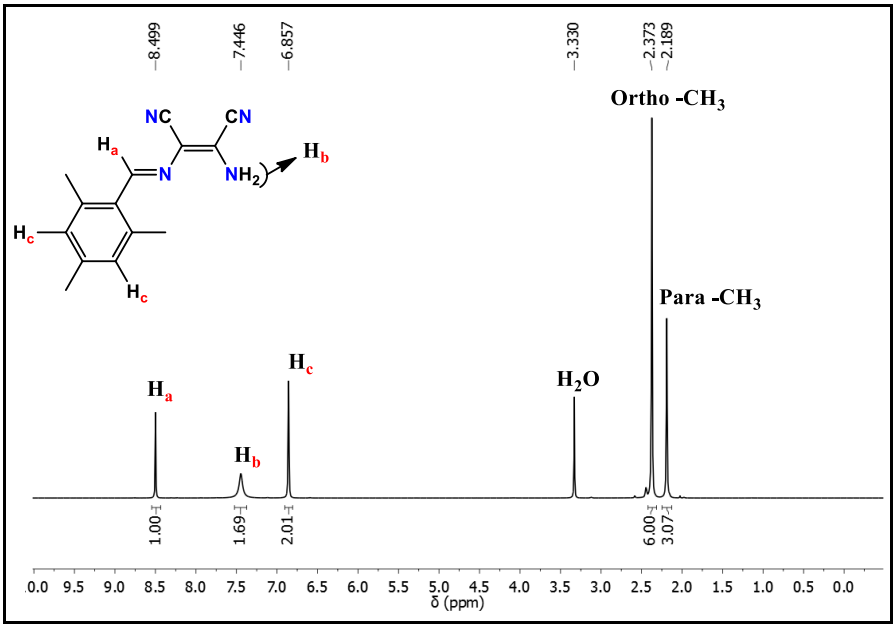


Figure S28: 1H NMR Spectrum of $\mathbf{C^{Mes}}$ in d_6-DMSO.

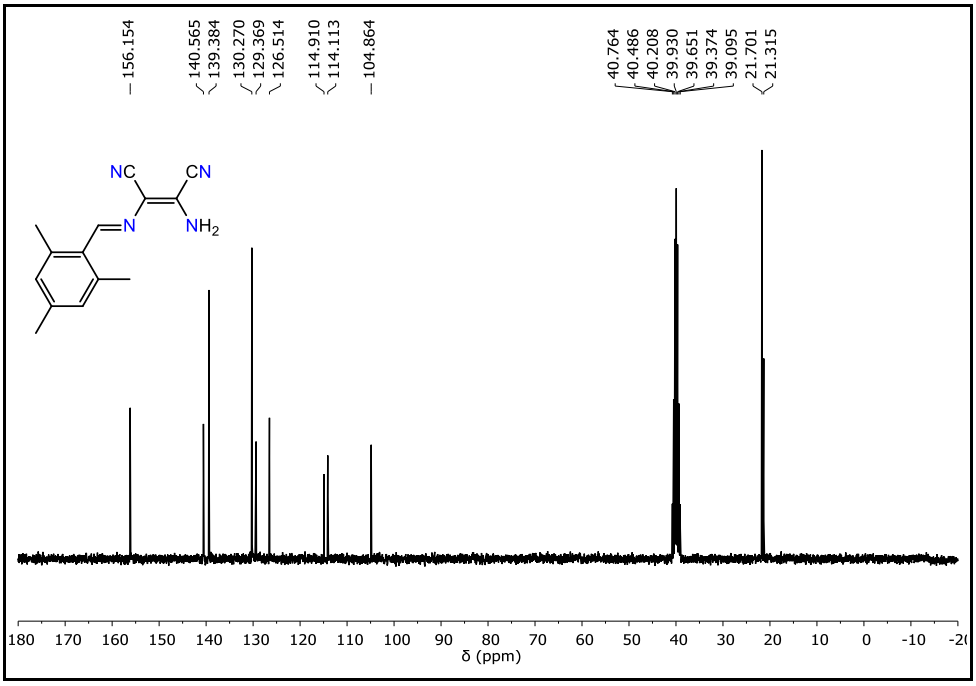


Figure S29: ^{13}C NMR Spectrum of $\mathbf{C}^{\mathbf{Mes}}$ in d_6-DMSO.

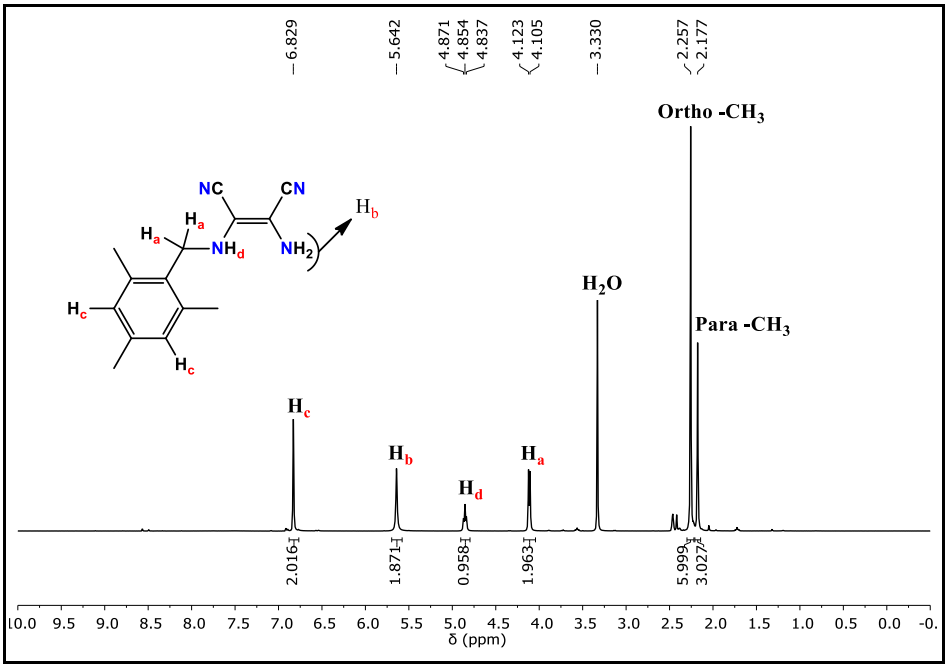


Figure S30: ^{1}H NMR Spectrum of $\mathbf{D}^{\mathbf{Mes}}$ in d_6-DMSO

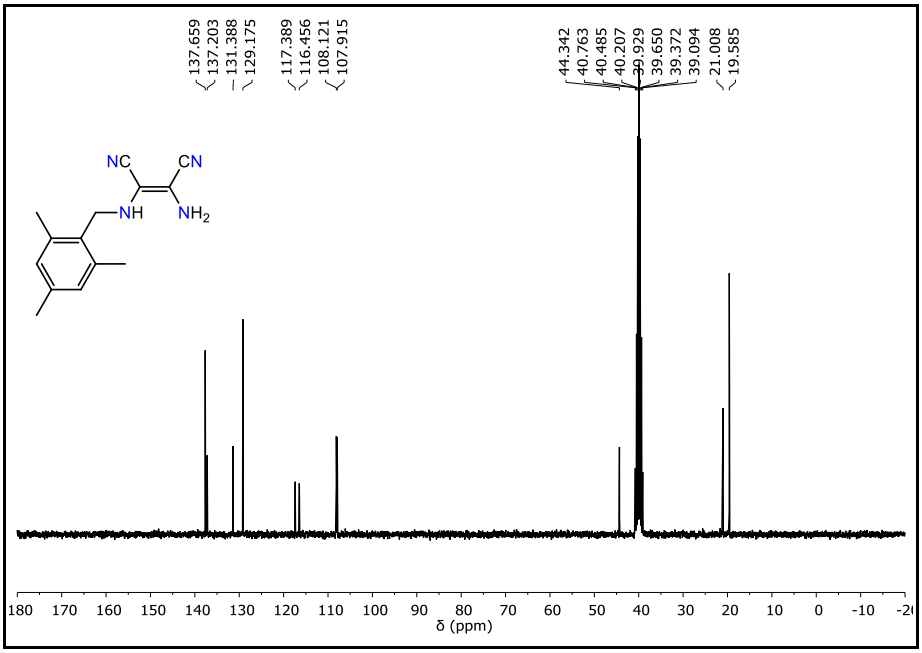


Figure S31: ^{13}C NMR Spectrum of $\mathbf{D^{Mes}}$ in d_6-DMSO.

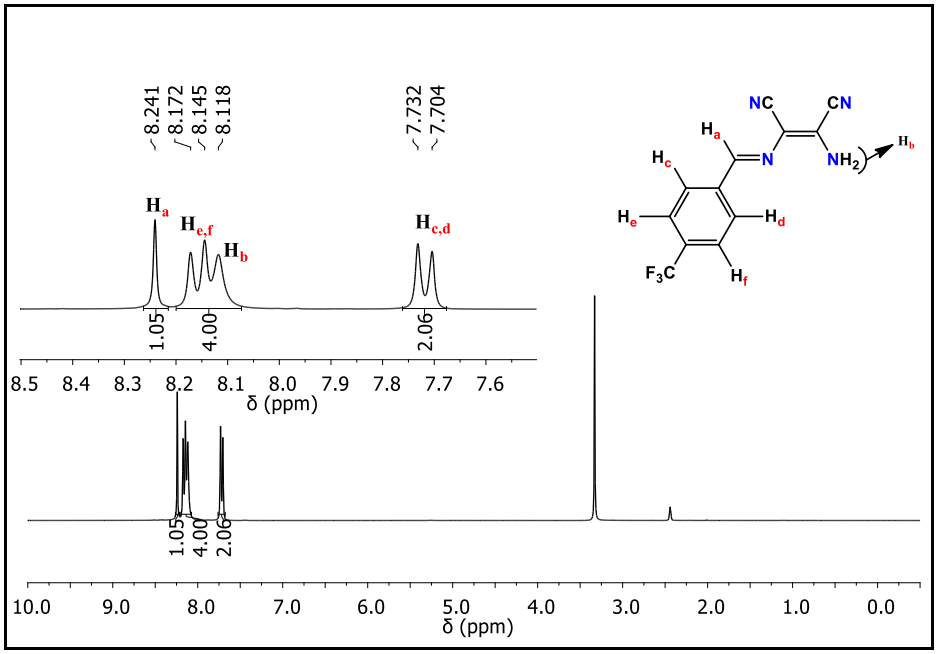


Figure S32: ^{1}H NMR Spectrum of $\mathbf{C^{CF3}}$ in d_6-DMSO

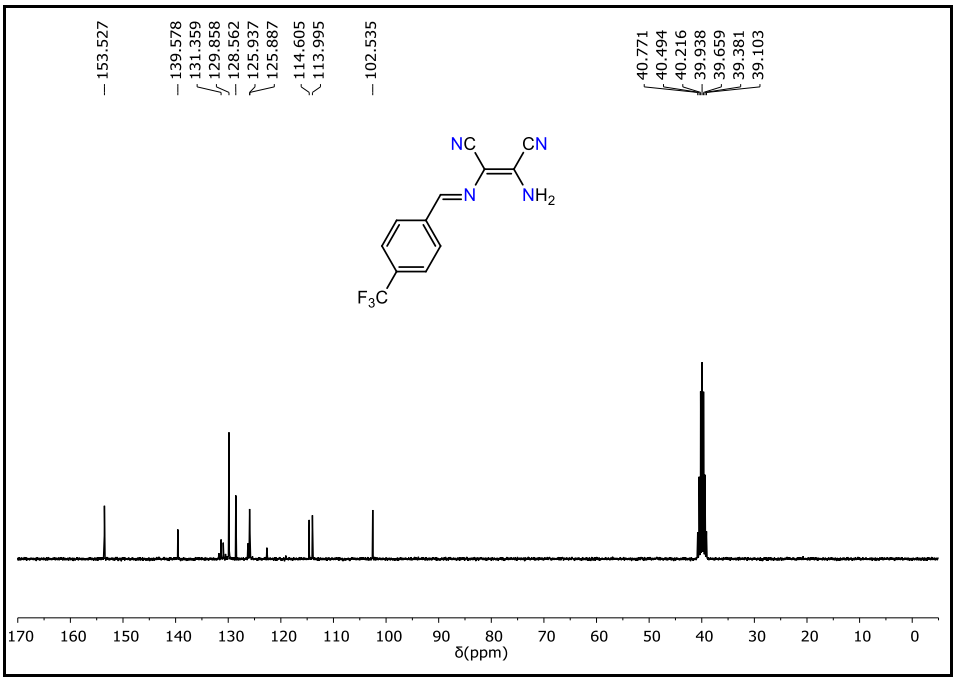


Figure S33: ^{13}C NMR Spectrum of $\mathbf{C^{CF3}}$ in d_6-DMSO

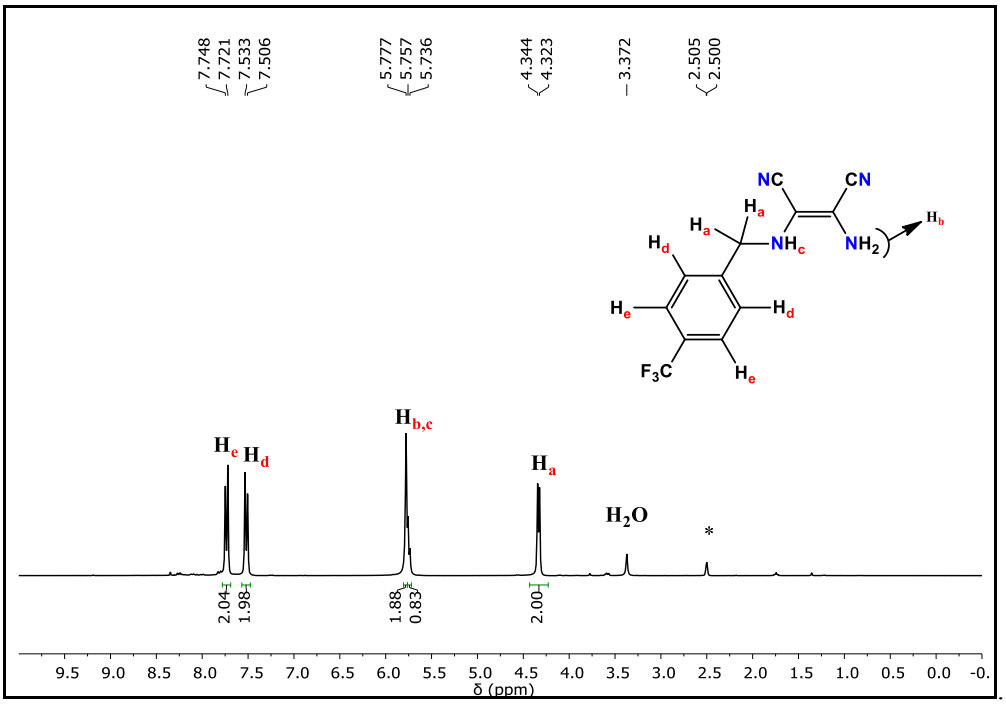


Figure S34: ^{1}H NMR Spectrum of $\mathbf{D}^{\mathbf{CF3}}$ in d_6-DMSO.

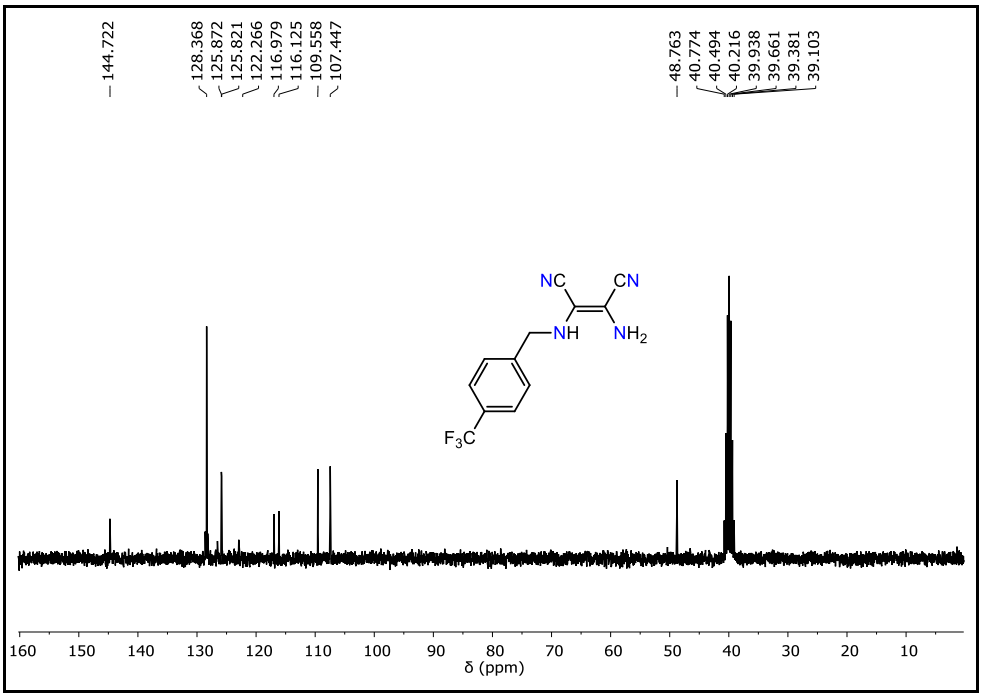


Figure S35: ^{13}C NMR Spectrum of $\mathbf{D}^{\mathbf{CF3}}$ in d_6-DMSO.

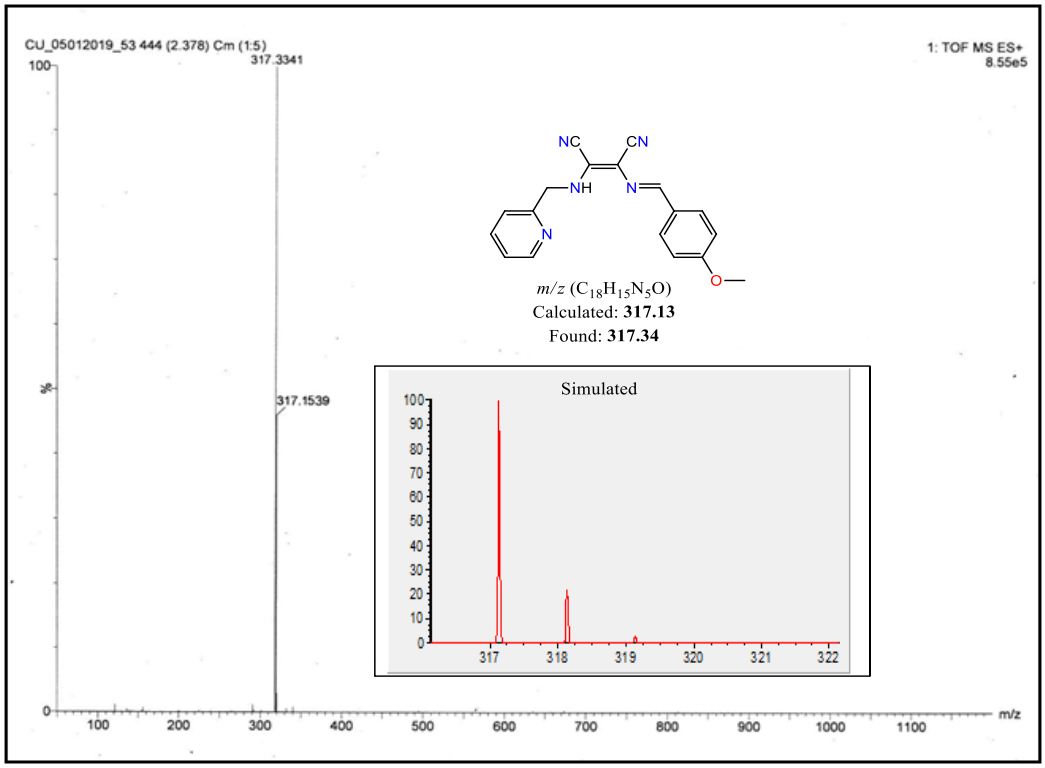


Figure S36: ESI-MS Spectrum of **HL**$^{\mathbf{1\text{-}OMe}}$.

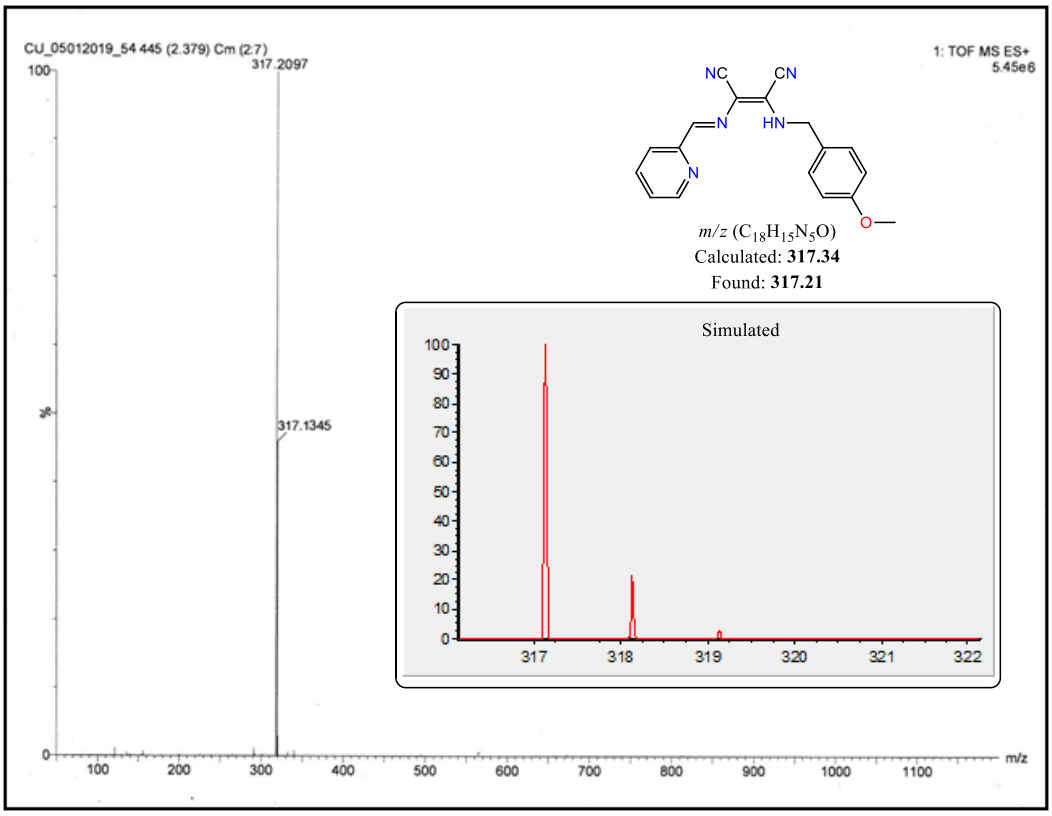


Figure S37: ESI-MS Spectrum of **HL**$^{\mathbf{2\text{-}OMe}}$.

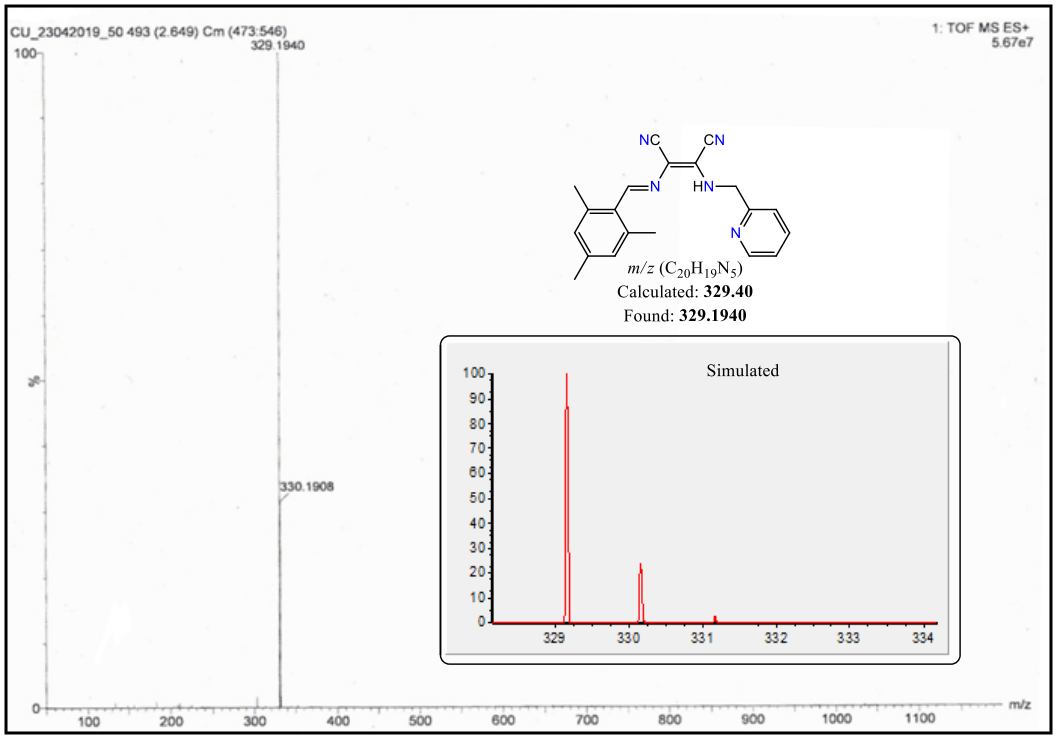


Figure S38: ESI-MS Spectrum of **HL**$^{\mathbf{1\text{-}Mes}}$.

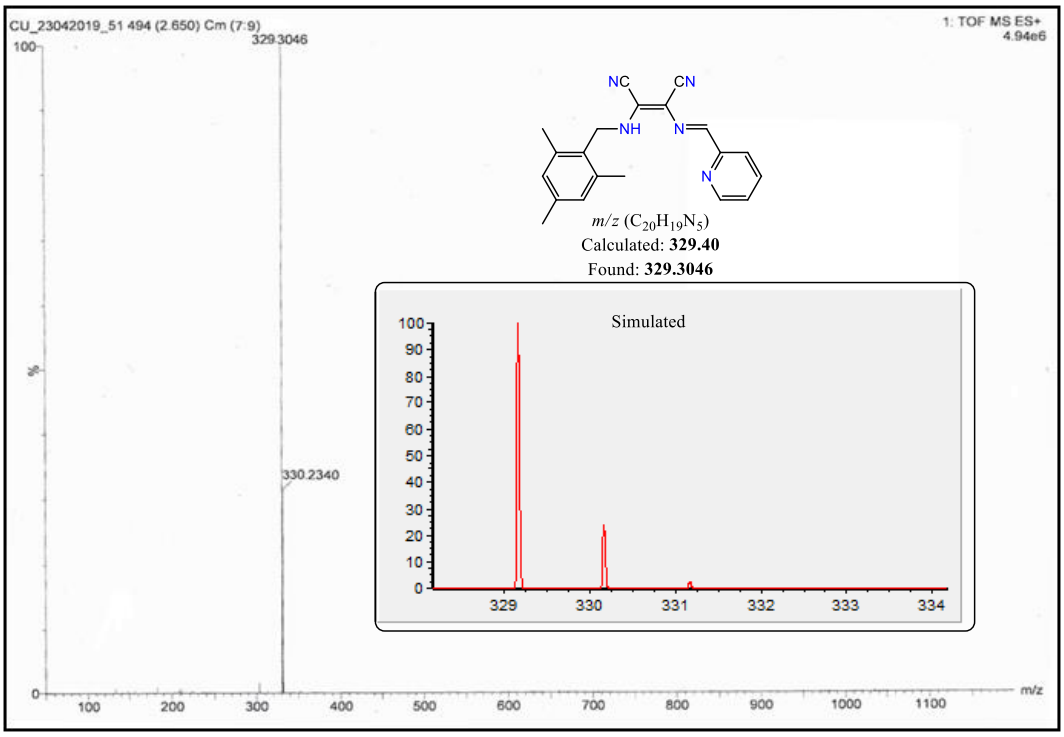


Figure S39: ESI-MS Spectrum of **HL**$^{\mathbf{2\text{-}Mes}}$.

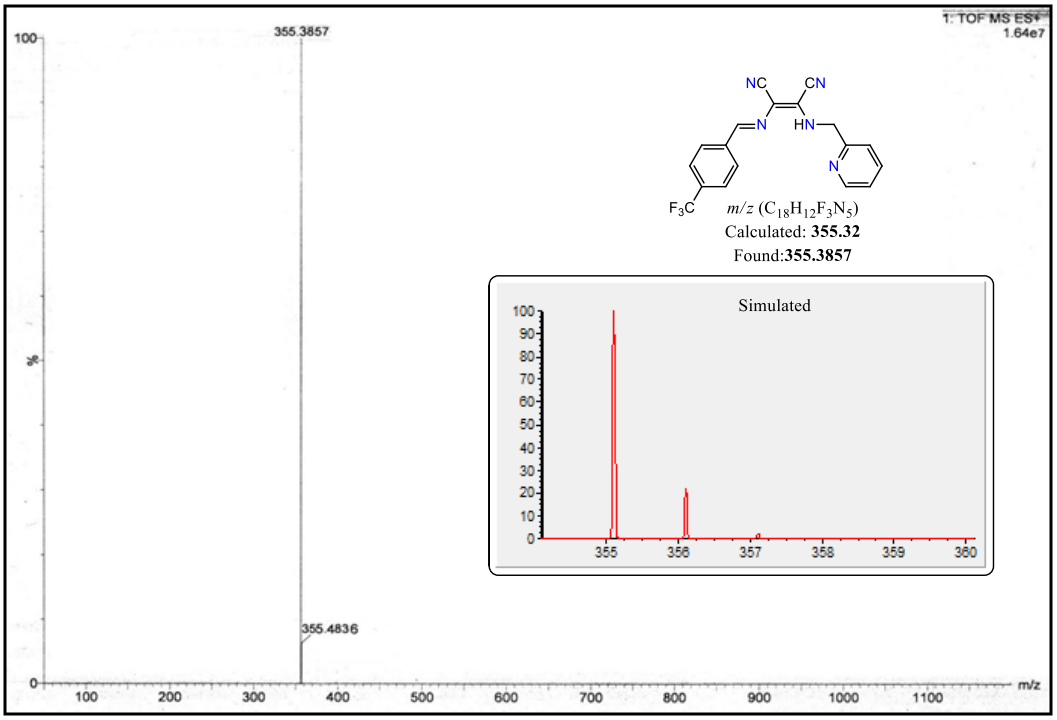


Figure S40: ESI-MS Spectrum of **HL**$^{1\text{-CF3}}$.

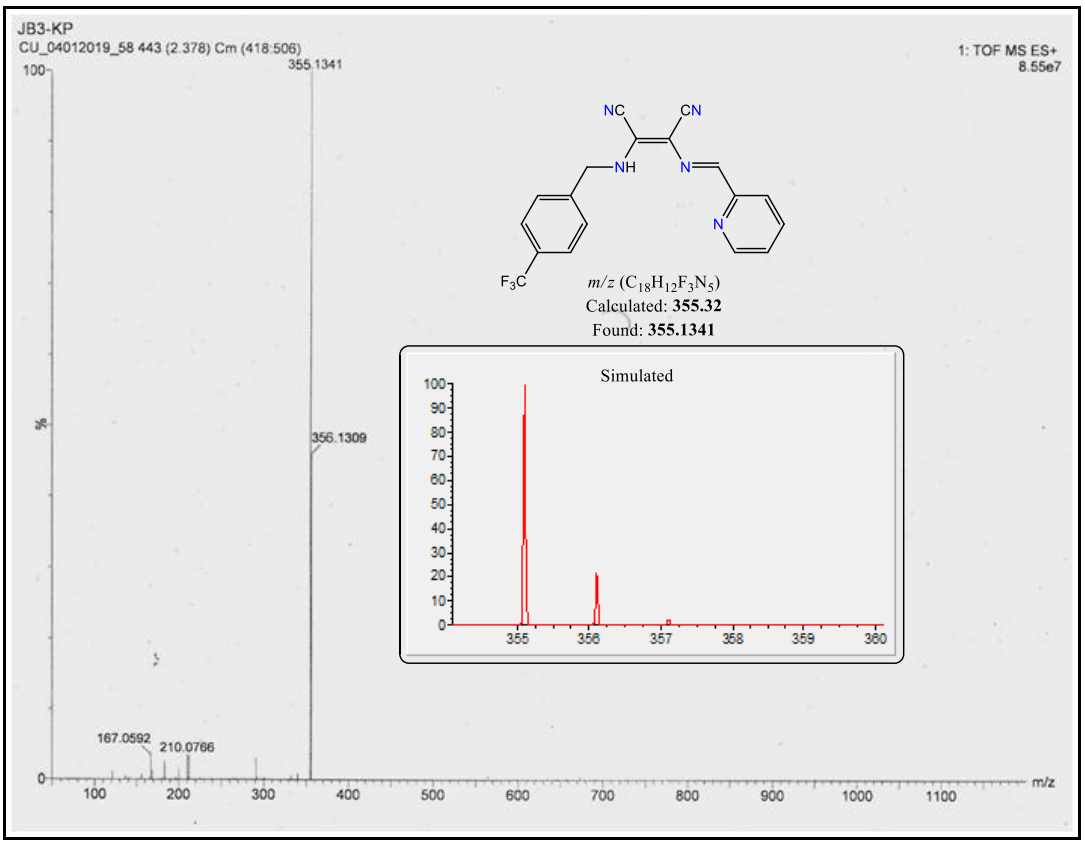


Figure S41: ESI-MS Spectrum of **HL**$^{2\text{-CF3}}$.

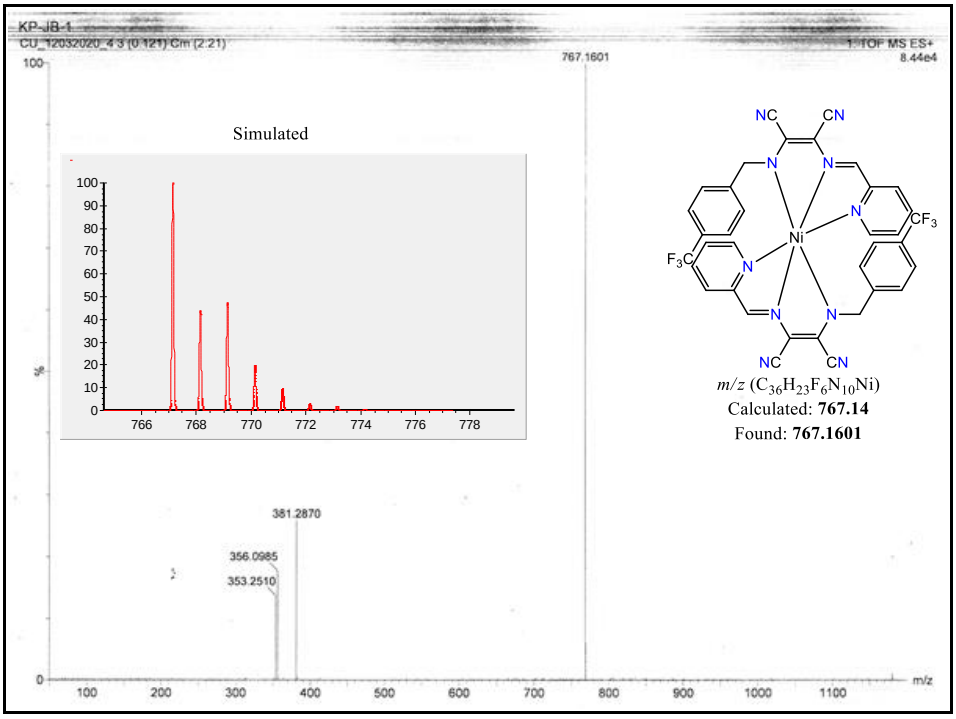


Figure S42: ESI-MS Spectrum of [(**Ni$^{2\text{-CF3}}$**) +**H$^+$**].

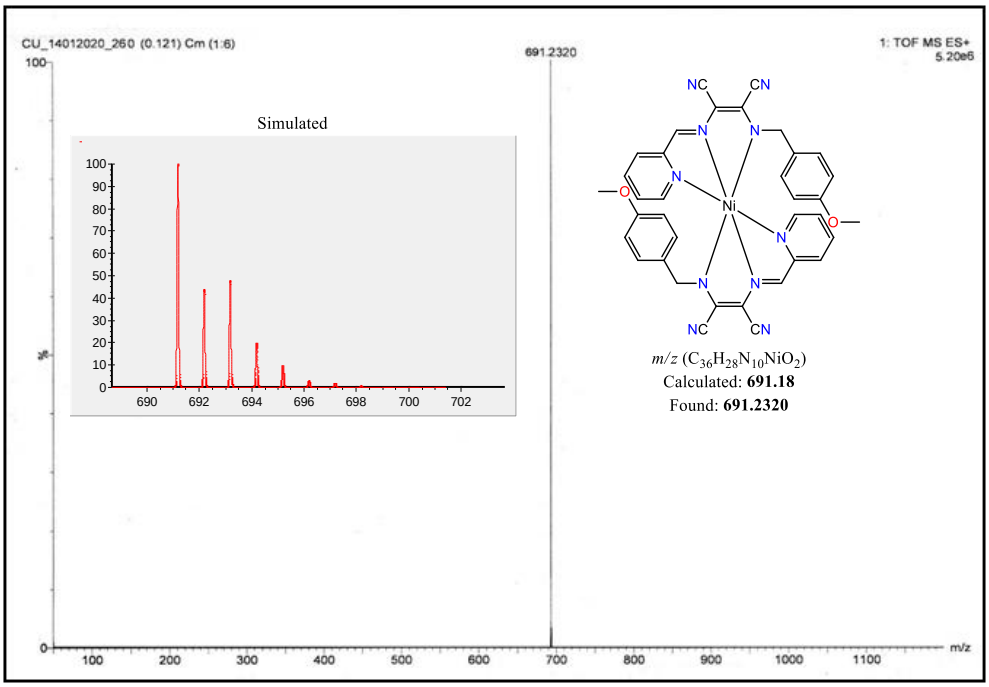


Figure S43: ESI-MS Spectrum of [(**Ni$^{2\text{-OMe}}$**)+**H$^+$**] .

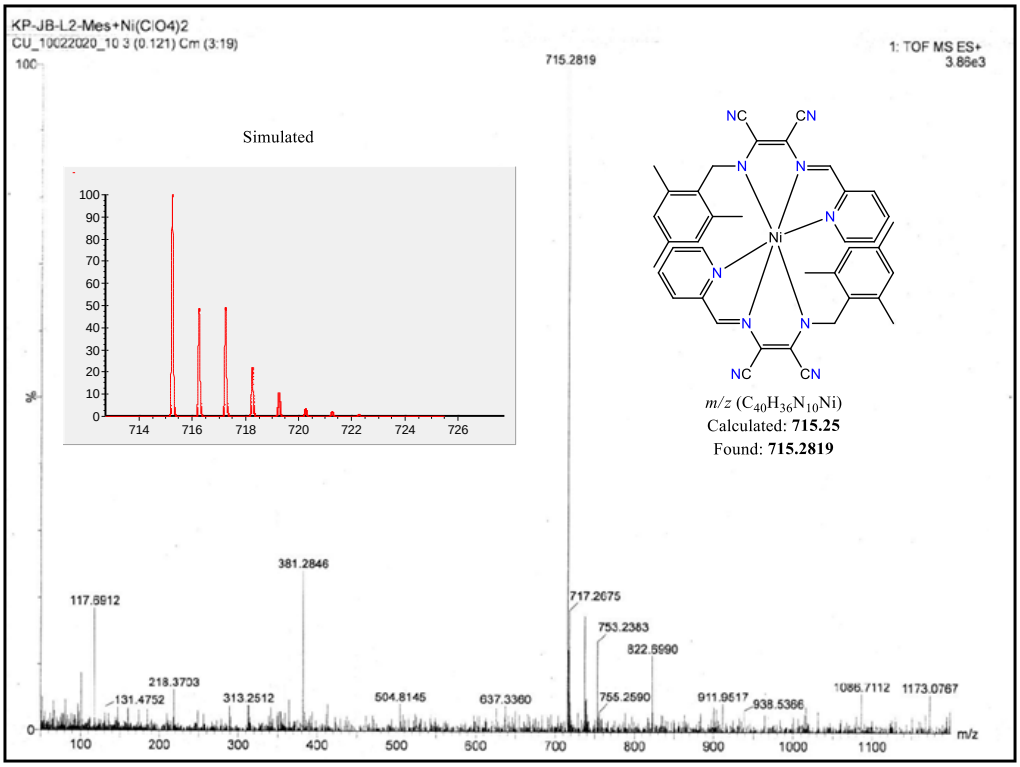


Figure S44: ESI-MS Spectrum of [($Ni^{2\text{-}Mes}$)+H^+].

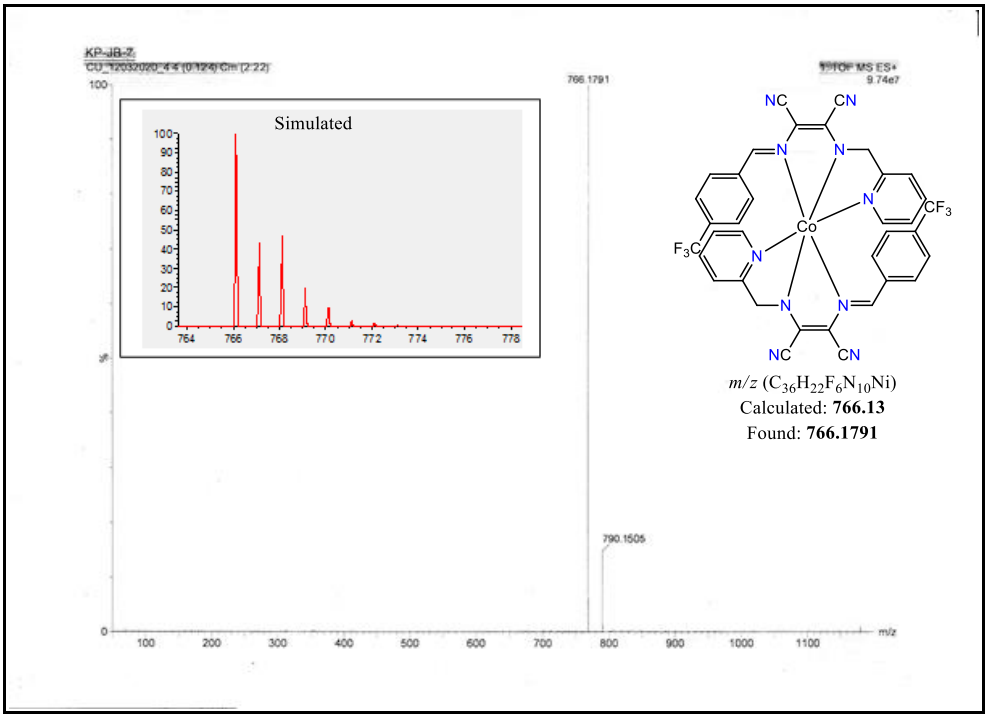


Figure S45: ESI-MS Spectrum of $Co^{1\text{-}CF3}$.

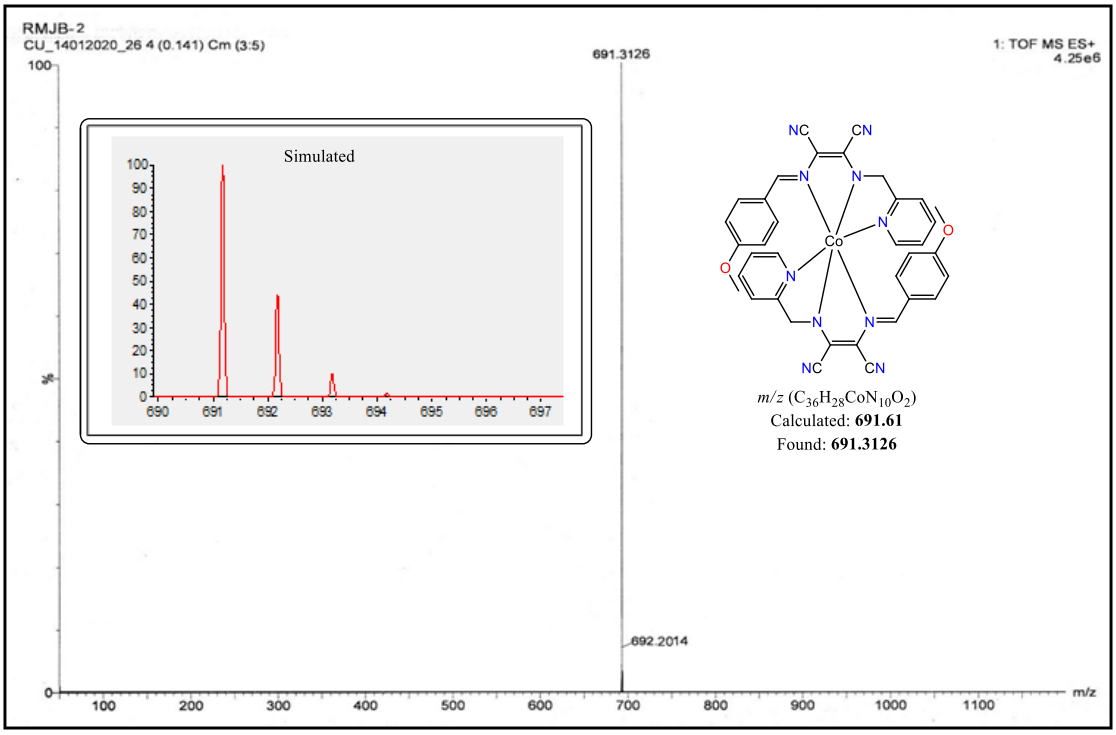


Figure S46: ESI-MS Spectrum of **Co**$^{\mathbf{1\text{-}OMe}}$.

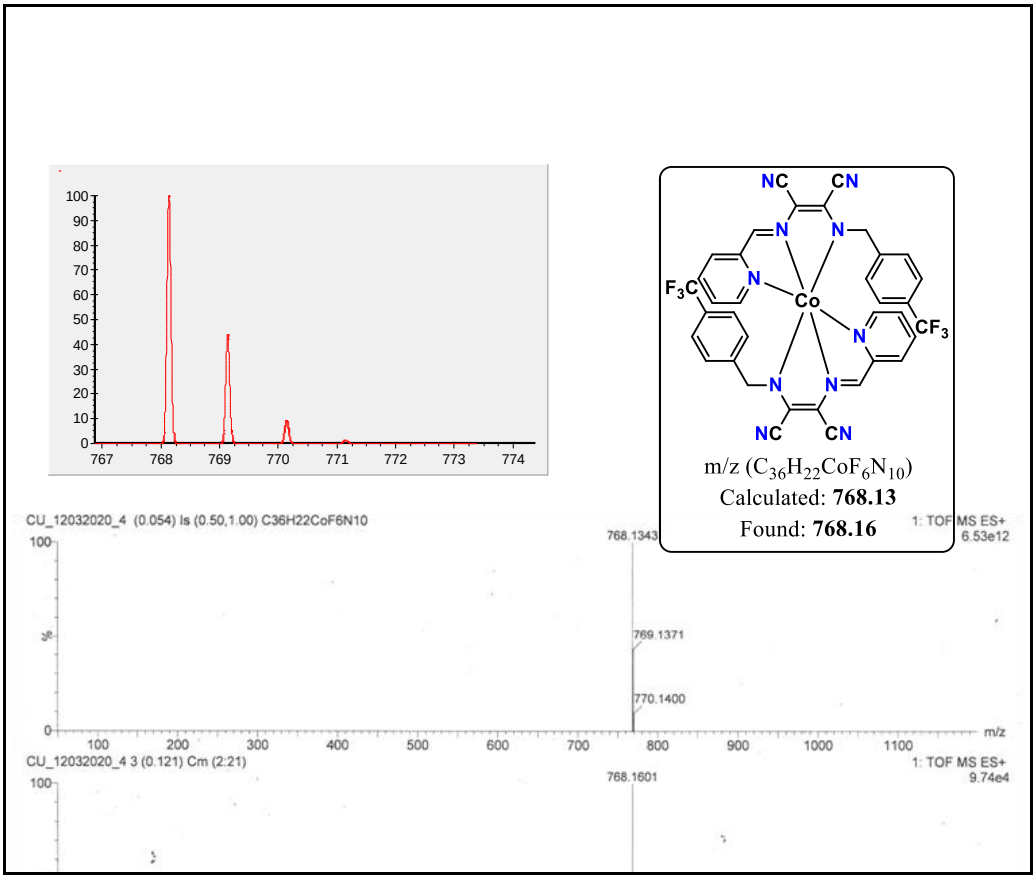


Figure S47: ESI-MS Spectrum of {[**Co**$^{\mathbf{2\text{-}CF3}}$**]+H**$^{+}$**}** (Ar-Prouct).

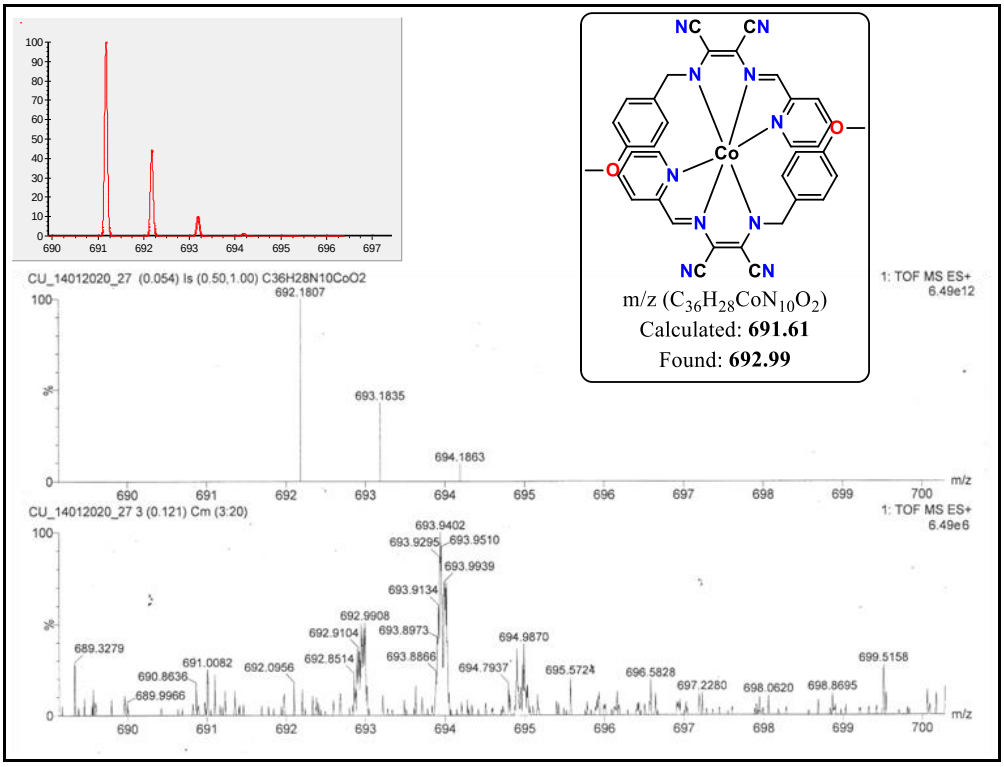


Figure S48: ESI-MS Spectrum of **$Co^{2\text{-}OMe}$** (Ar-Prouct).

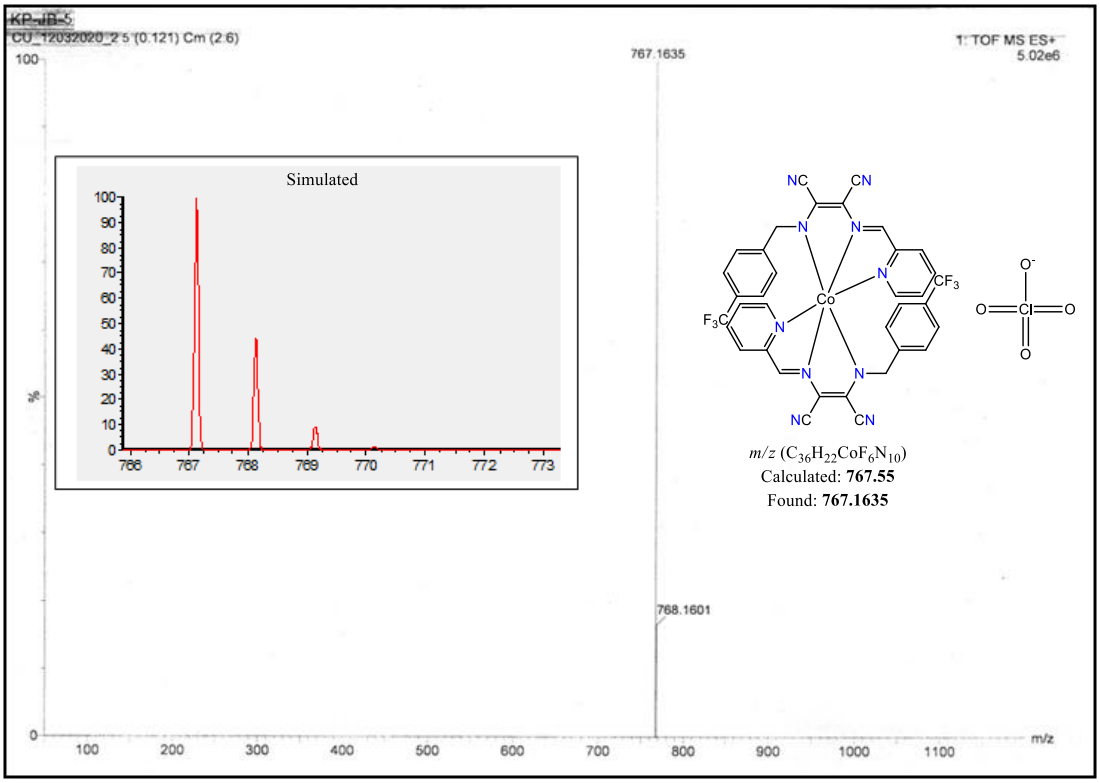


Figure S49: ESI-MS Spectrum of **$Co^{2\text{-}CF3}.ClO_4$**.

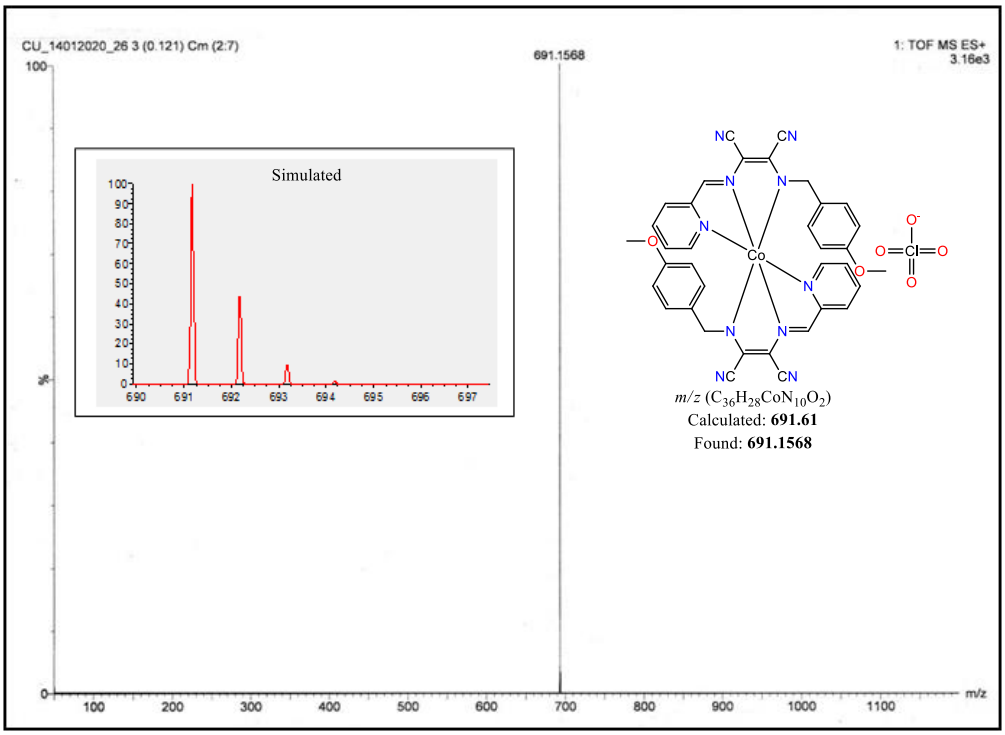


Figure S50: ESI-MS Spectrum of $\mathbf{Co^{2\text{-}OMe}.ClO_4}$.

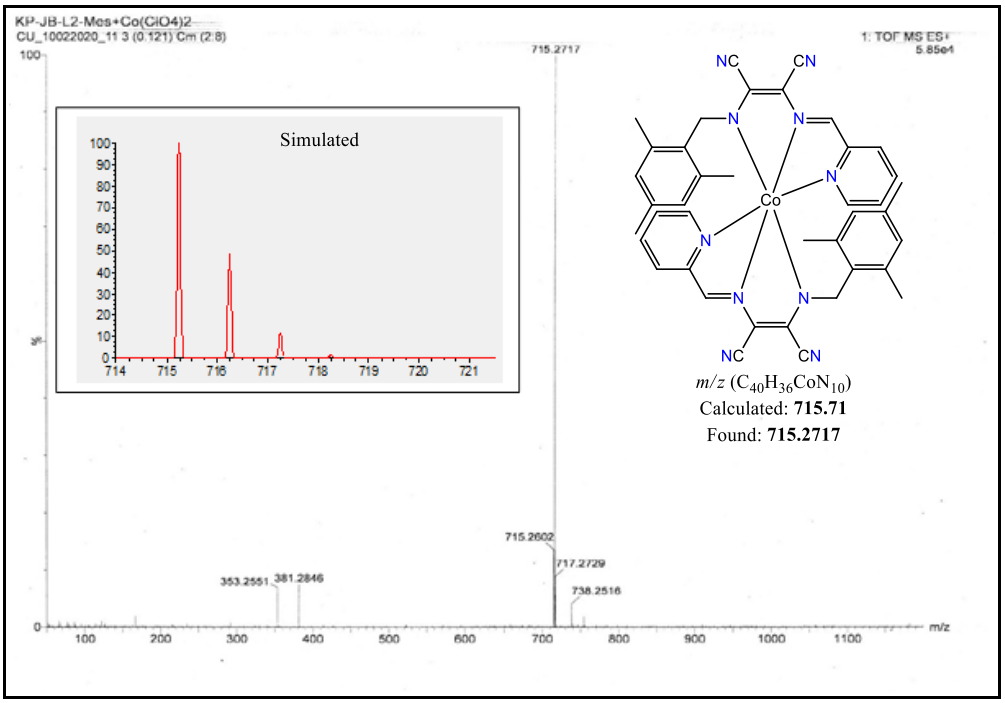


Figure S51: ESI-MS Spectrum of $\mathbf{Co^{2\text{-}Mes}}$

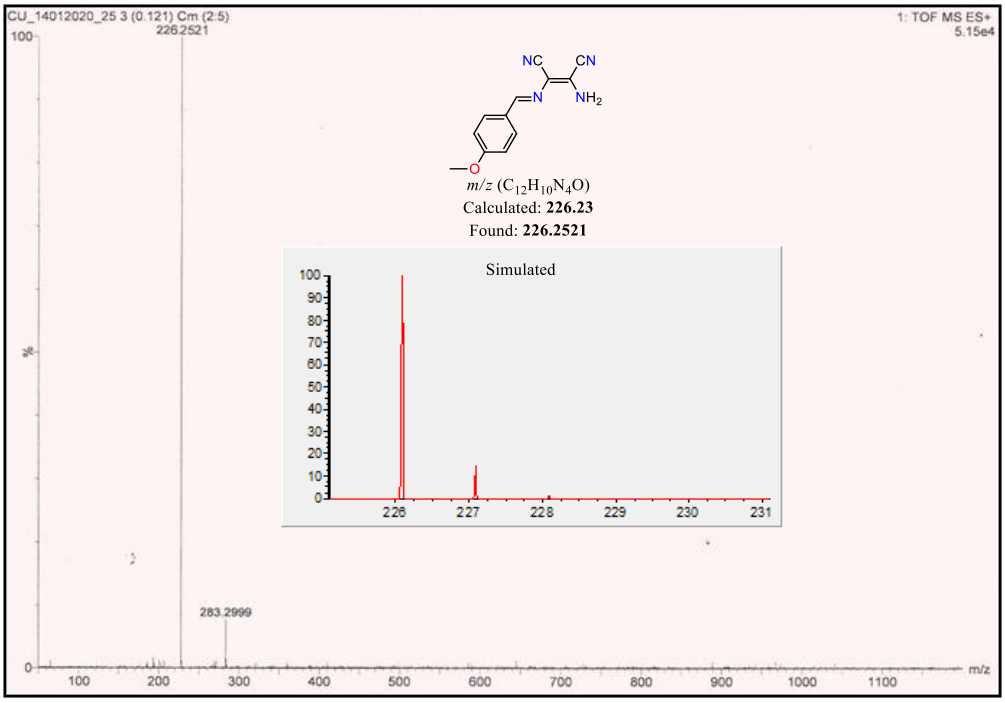


Figure S52: ESI-MS Spectrum of $\mathbf{C}^{\mathbf{OMe}}$.

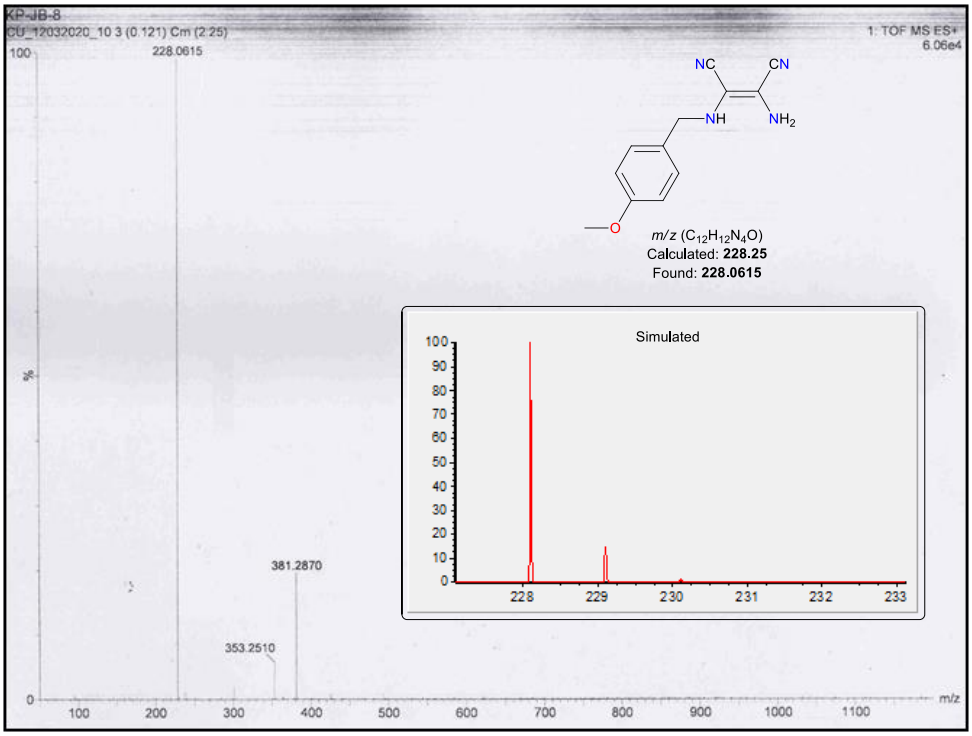


Figure S53: ESI-MS Spectrum of $\mathbf{D}^{\mathbf{OMe}}$.

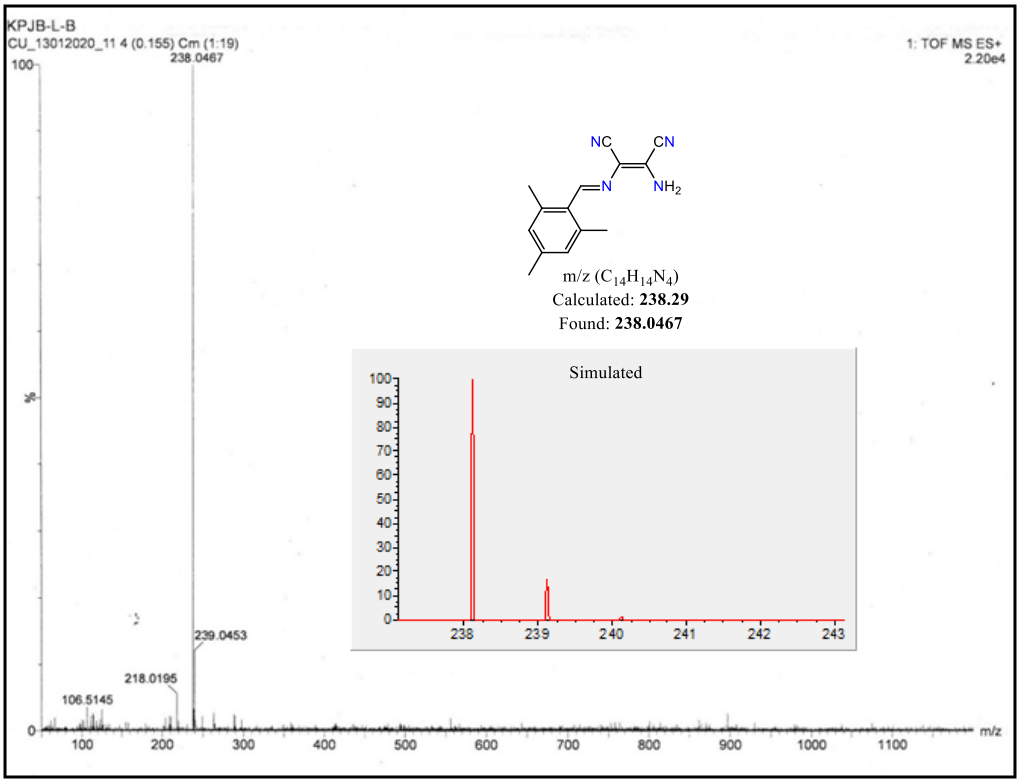


Figure S54: ESI-MS Spectrum of $\mathbf{C}^{\mathbf{Mes}}$.

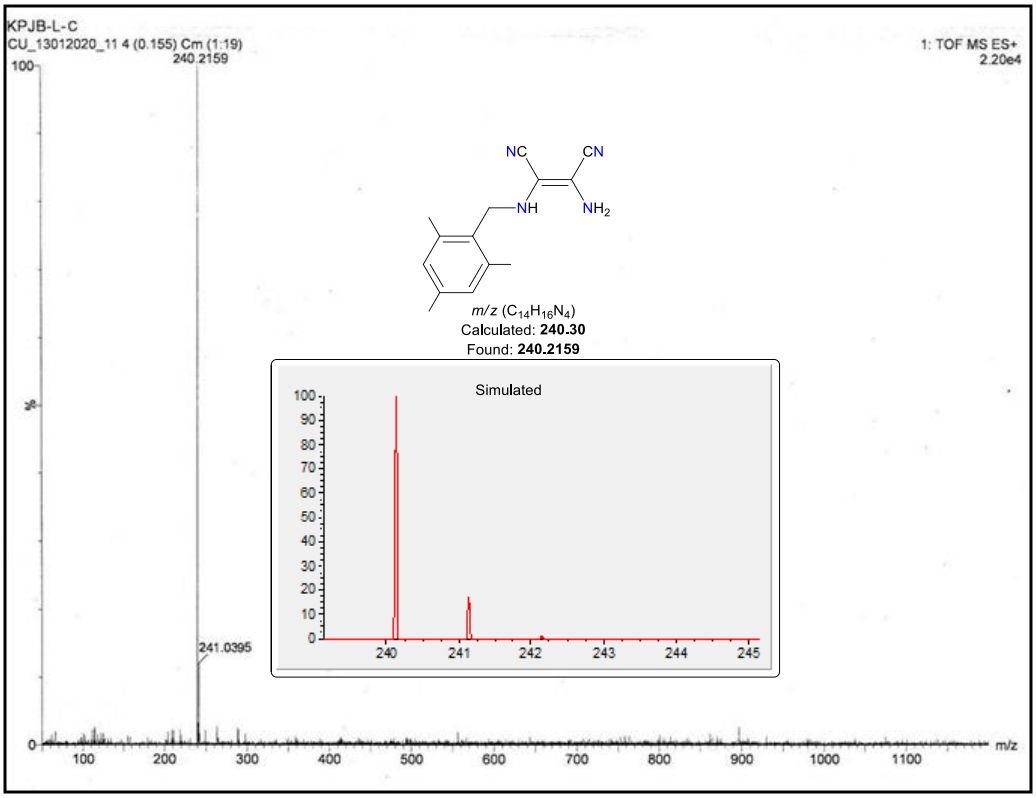


Figure S55: ESI-MS Spectrum of $\mathbf{D}^{\mathbf{Mes}}$.

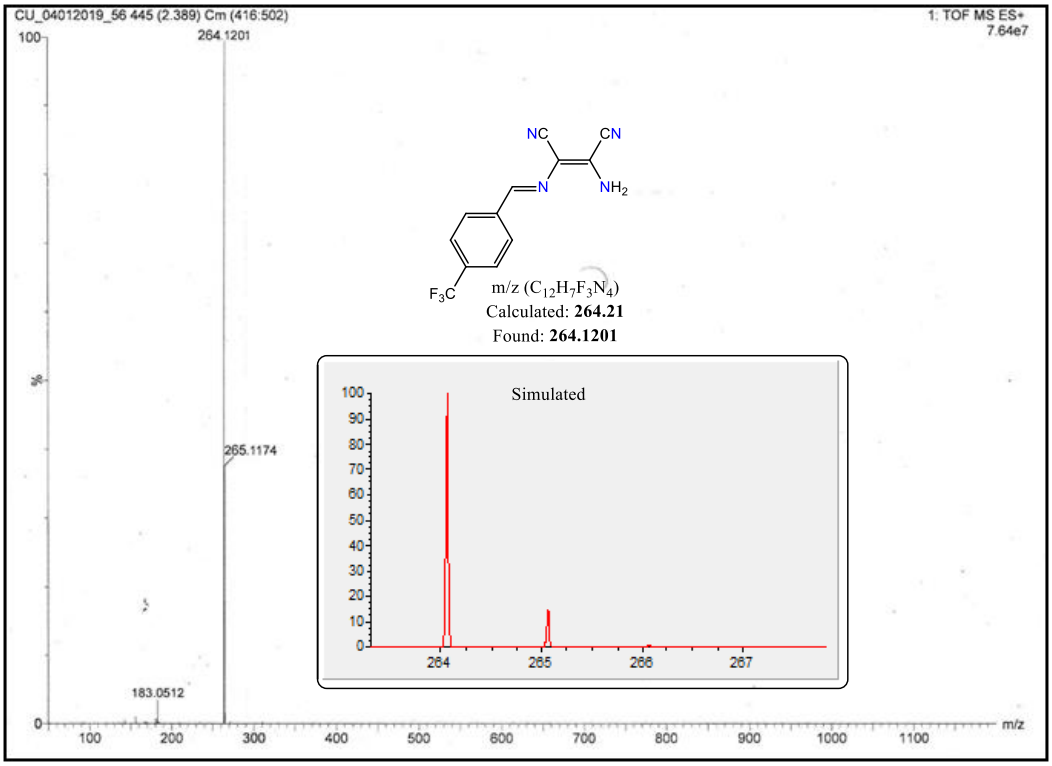


Figure S56: ESI-MS Spectrum of $\mathbf{C}^{\mathbf{CF3}}$

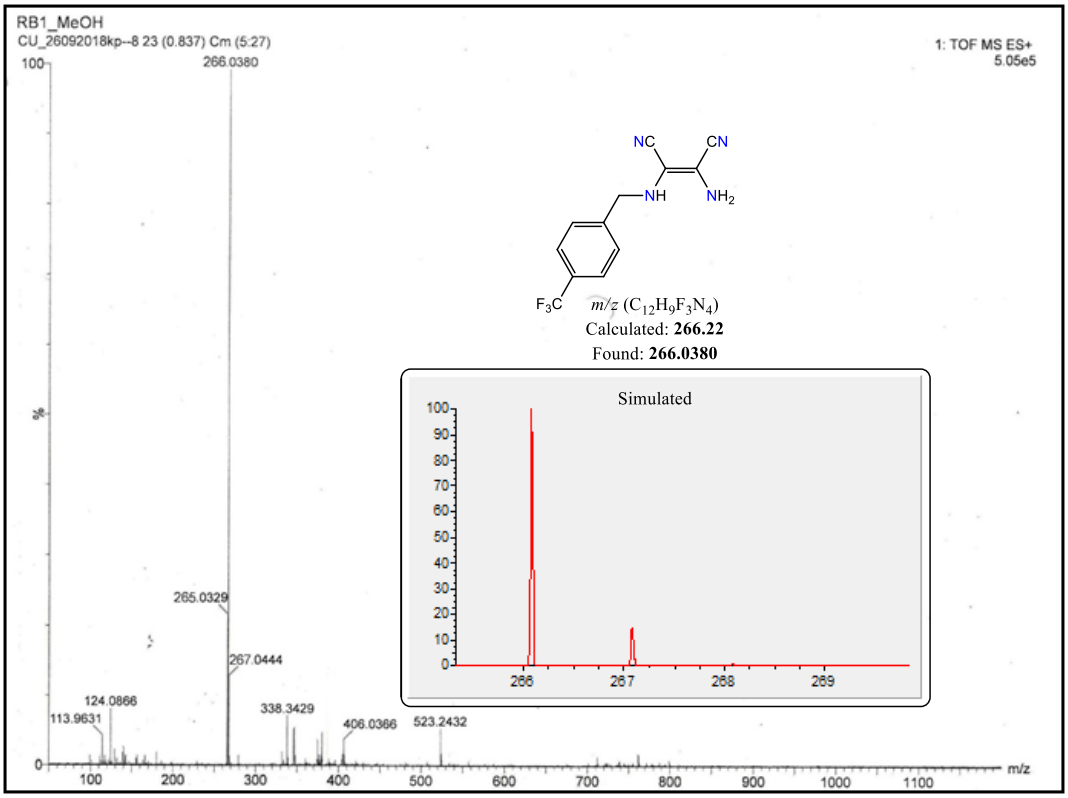


Figure S57: ESI-MS Spectrum of $\mathbf{D}^{\mathbf{CF3}}$.

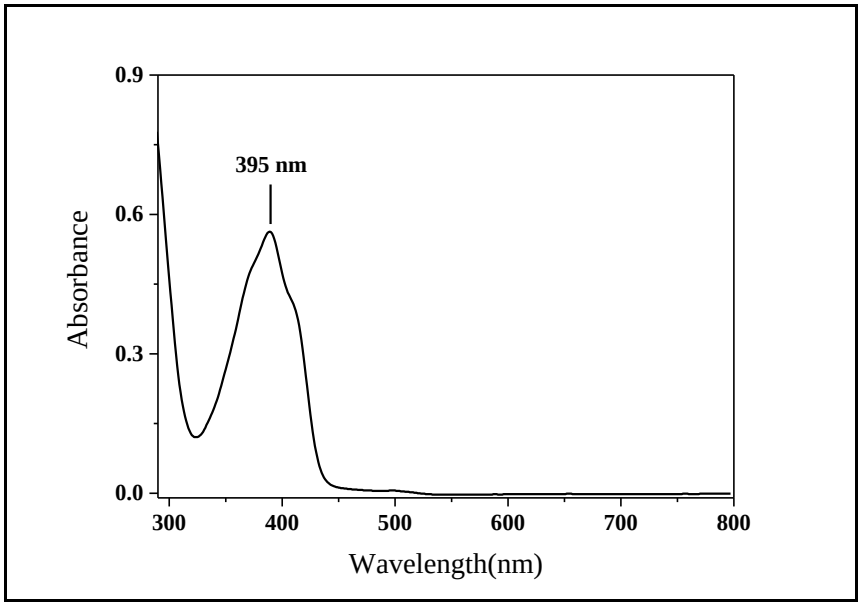


Figure S58: Electronic absorption spectra of **HL**$^{\mathbf{1\text{-}OMe}}$ (1 x 10^{-5}(M) in DMF

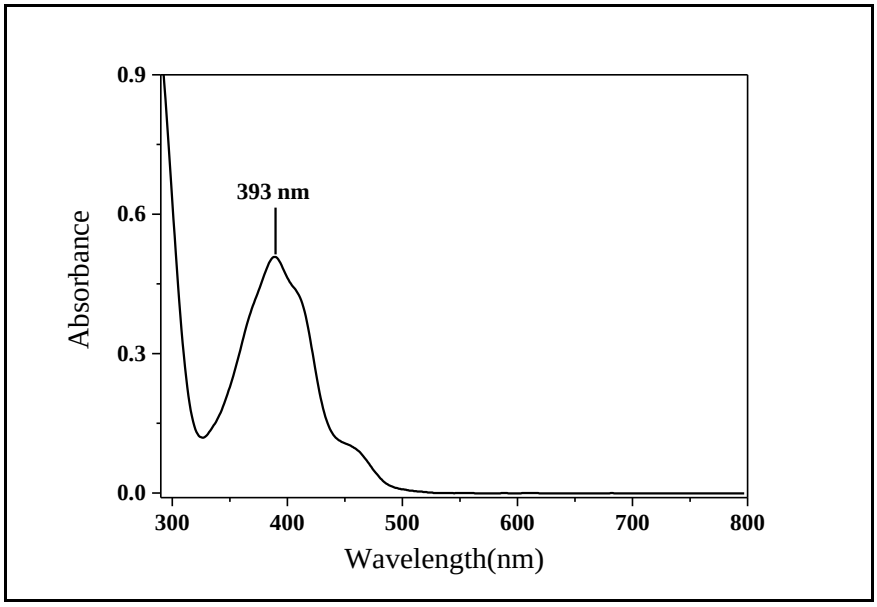


Figure S59: Electronic absorption spectra of **HL**$^{\mathbf{1\text{-}CF3}}$ (1 x 10^{-5}(M) in DMF

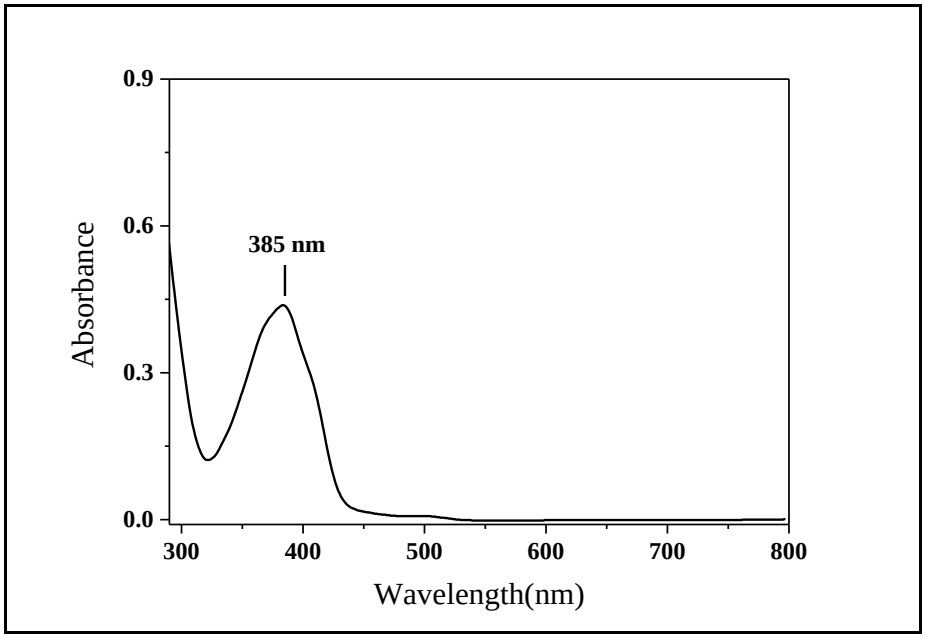


Figure S60: Electronic absorption spectra of **HL**$^{\mathbf{1\text{-}Mes}}$ (1 x 10^{-5}(M) in DMF

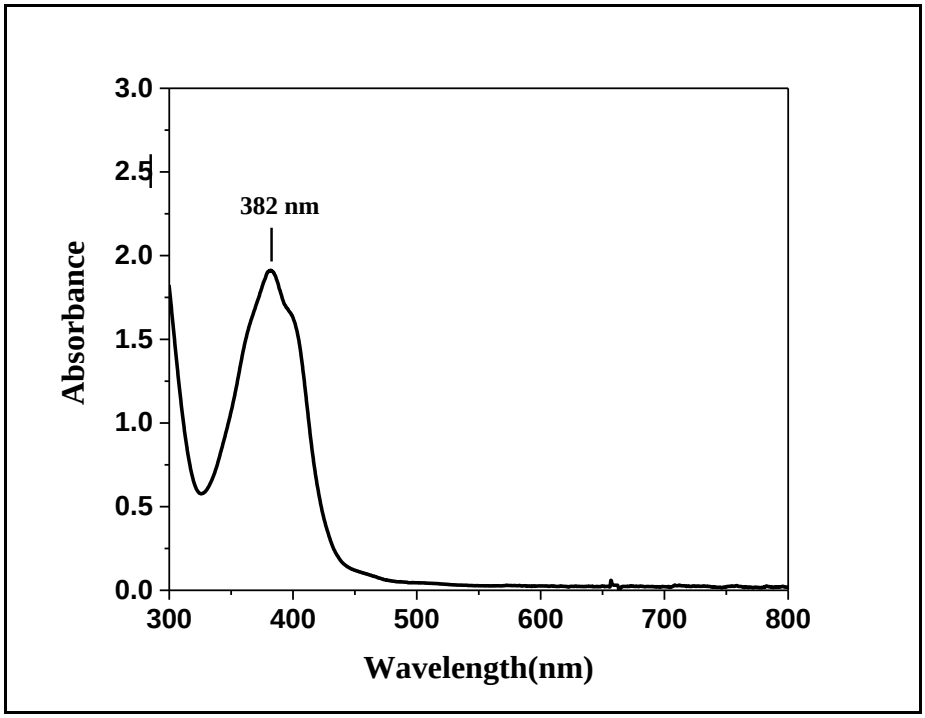


Figure S61: Electronic absorption spectra of **HL**$^{\mathbf{2\text{-}OMe}}$ (3.4 x 10^{-5}(M) in DMF

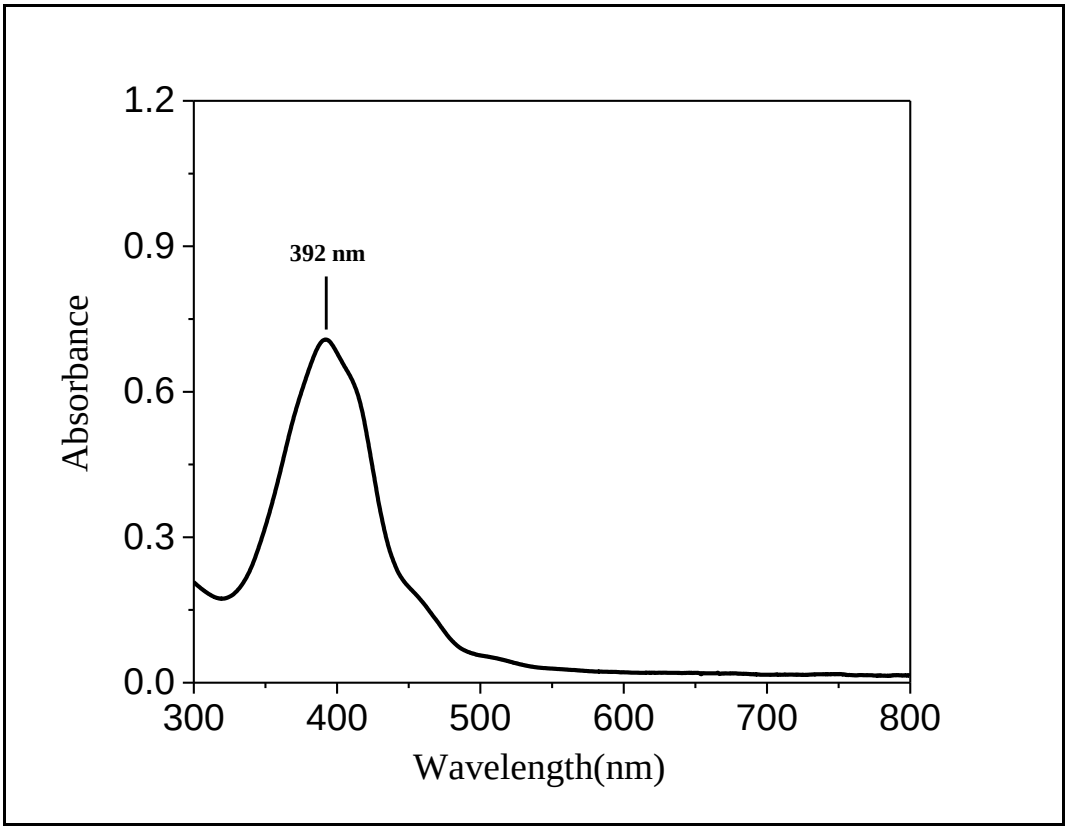


Figure S62: Electronic absorption spectra of $\mathbf{HL^{2\text{-}CF3}}$ (1.3×10^{-5}(M) in DMF

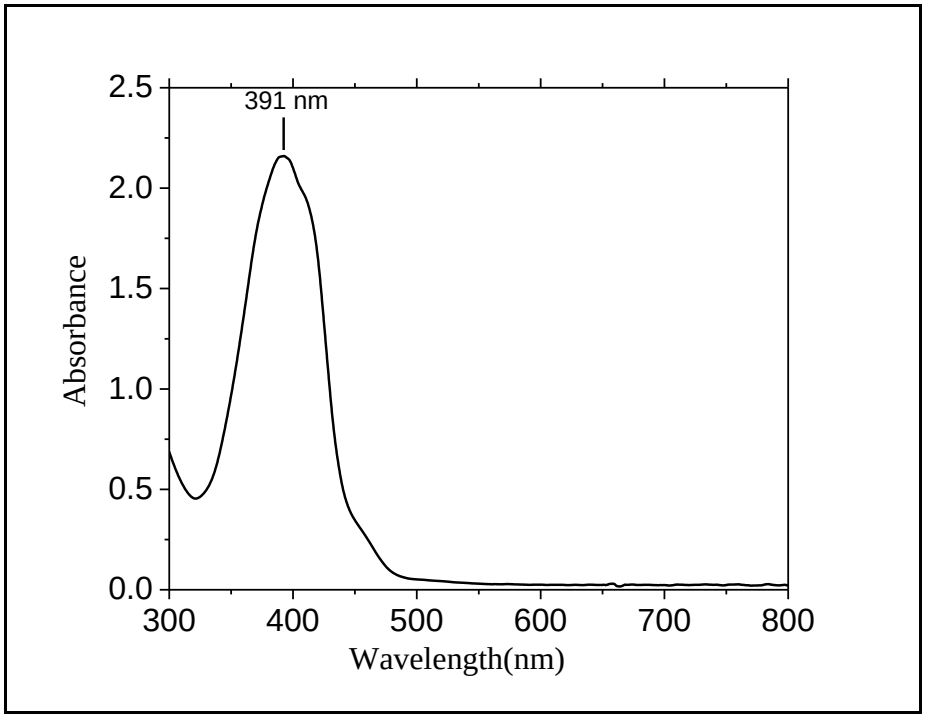


Figure S63: Electronic absorption spectra of $\mathbf{HL^{2\text{-}Mes}}$ (4.9×10^{-5}(M) in DMF

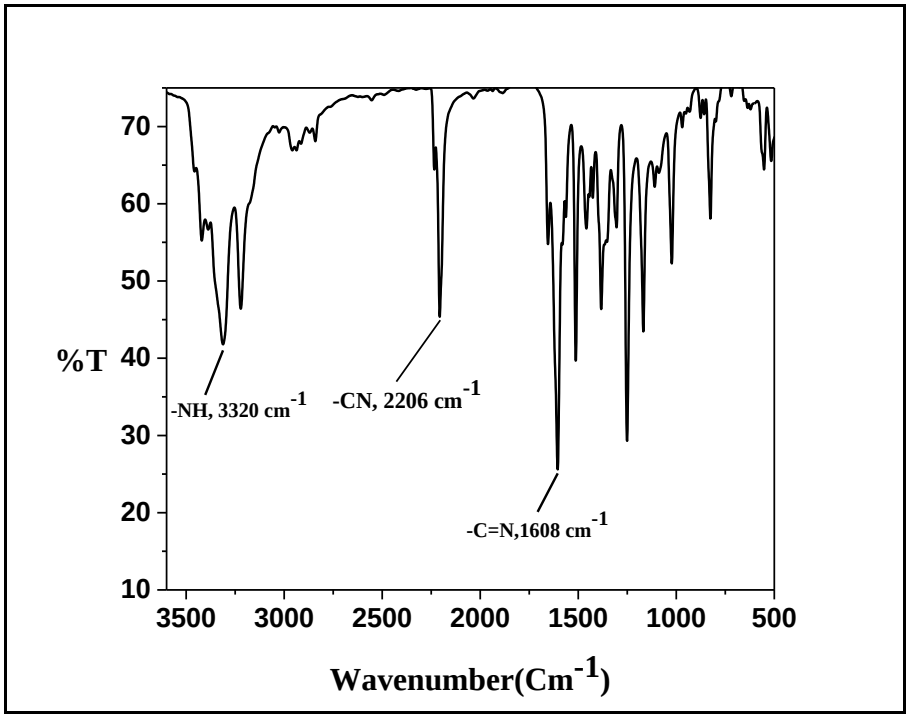


Figure S64: FTIR Spectrum of $\mathbf{HL}^{\mathbf{1\text{-}OMe}}$.

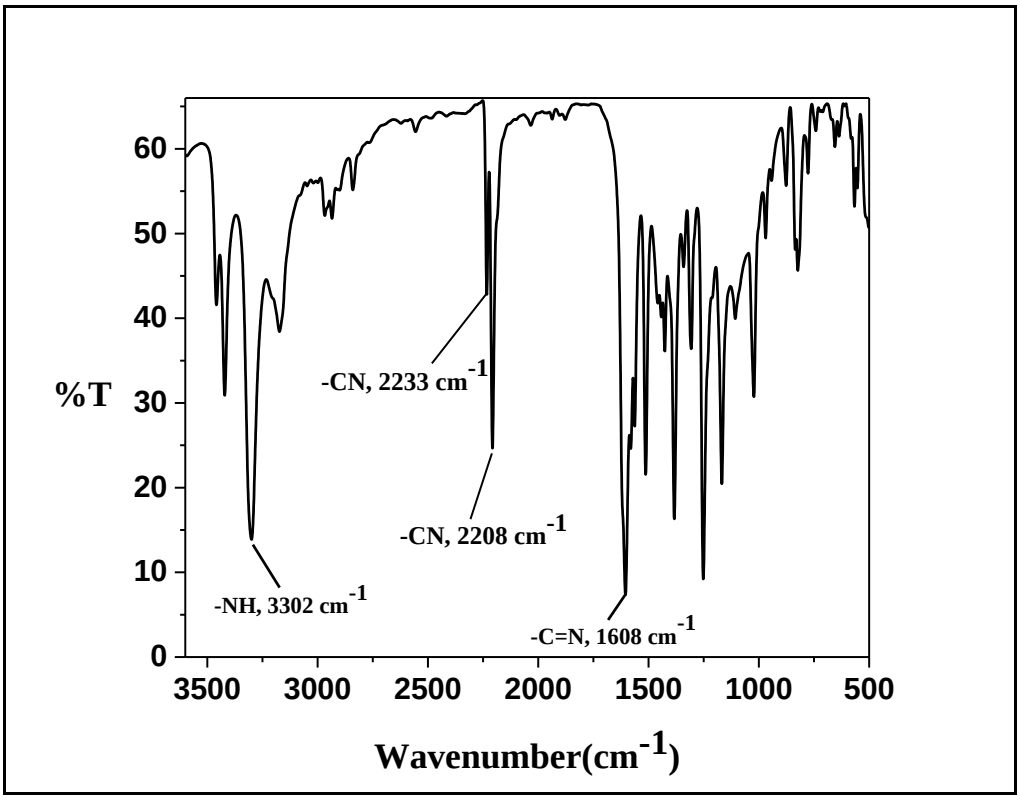


Figure S65: FTIR Spectrum of $\mathbf{HL}^{\mathbf{2\text{-}OMe}}$.

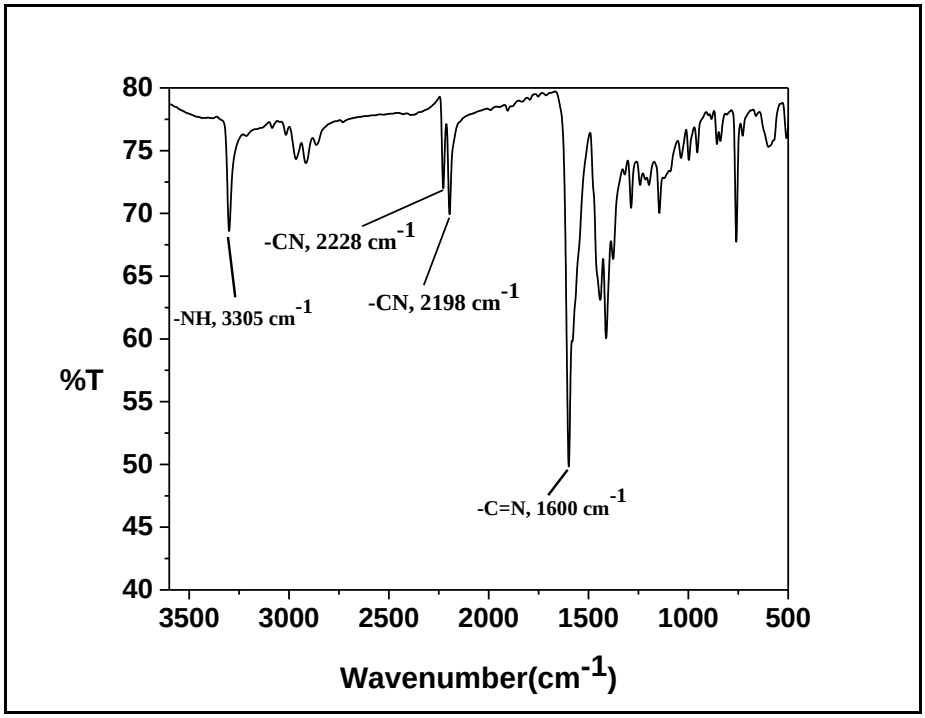


Figure S66: FTIR Spectrum of $\mathbf{HL}^{\mathbf{1\text{-}Mes}}$.

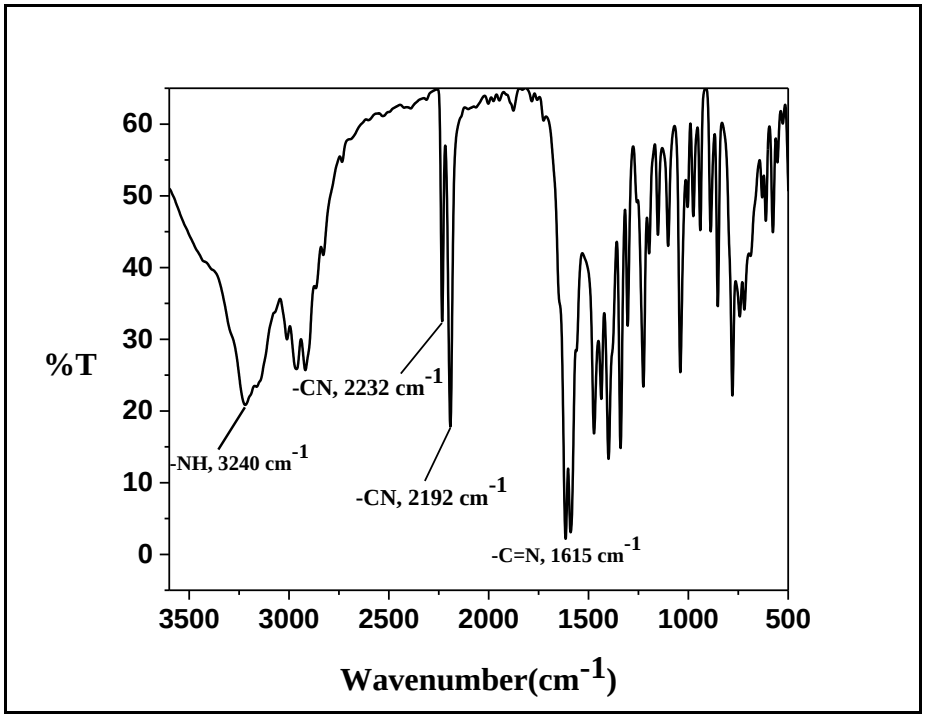


Figure S67: FTIR Spectrum of $\mathbf{HL}^{\mathbf{2\text{-}Mes}}$.

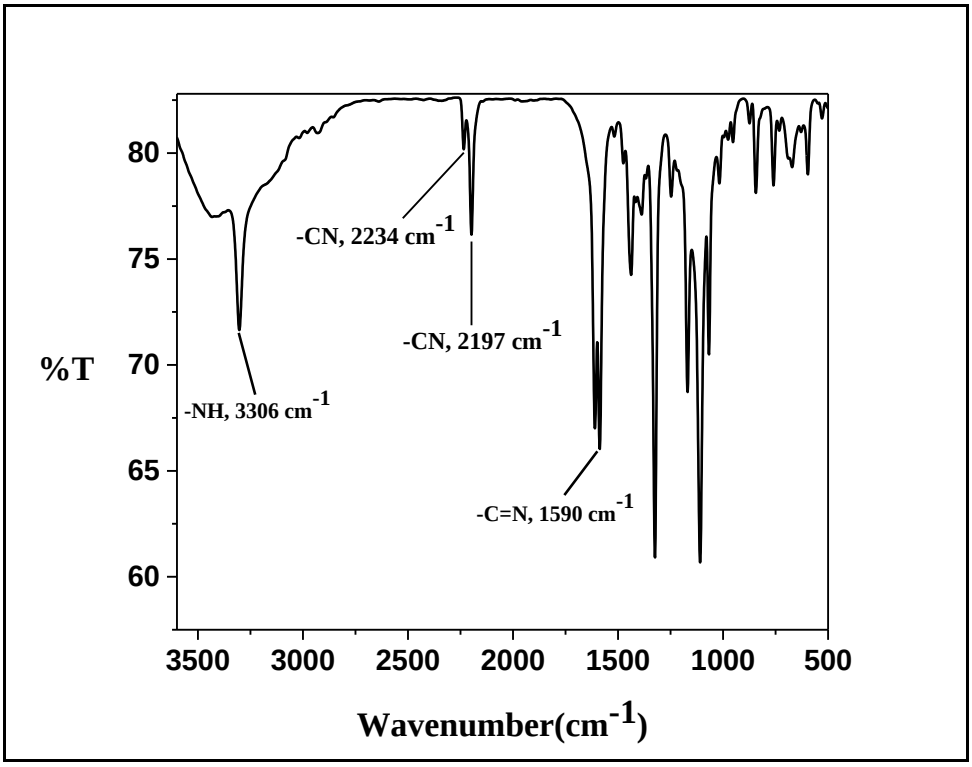


Figure S68: FTIR Spectrum of $\mathbf{HL}^{\mathbf{1\text{-}CF3}}$.

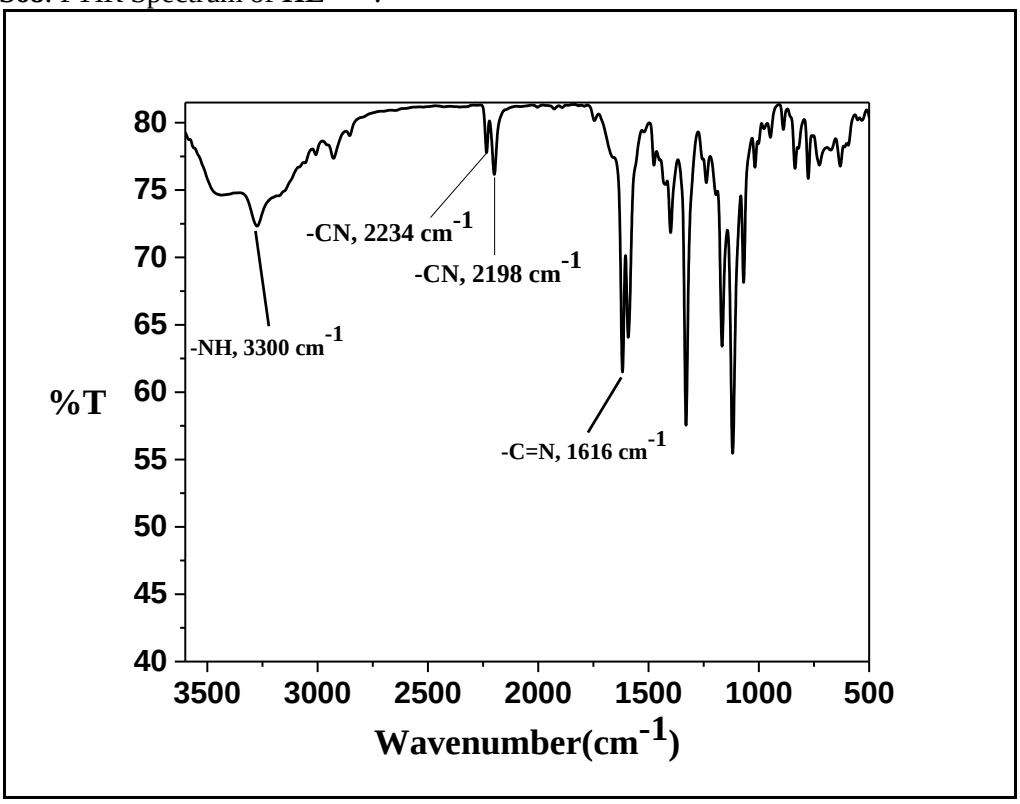


Figure S69: FTIR Spectrum of $\mathbf{HL}^{\mathbf{2\text{-}CF3}}$**.**

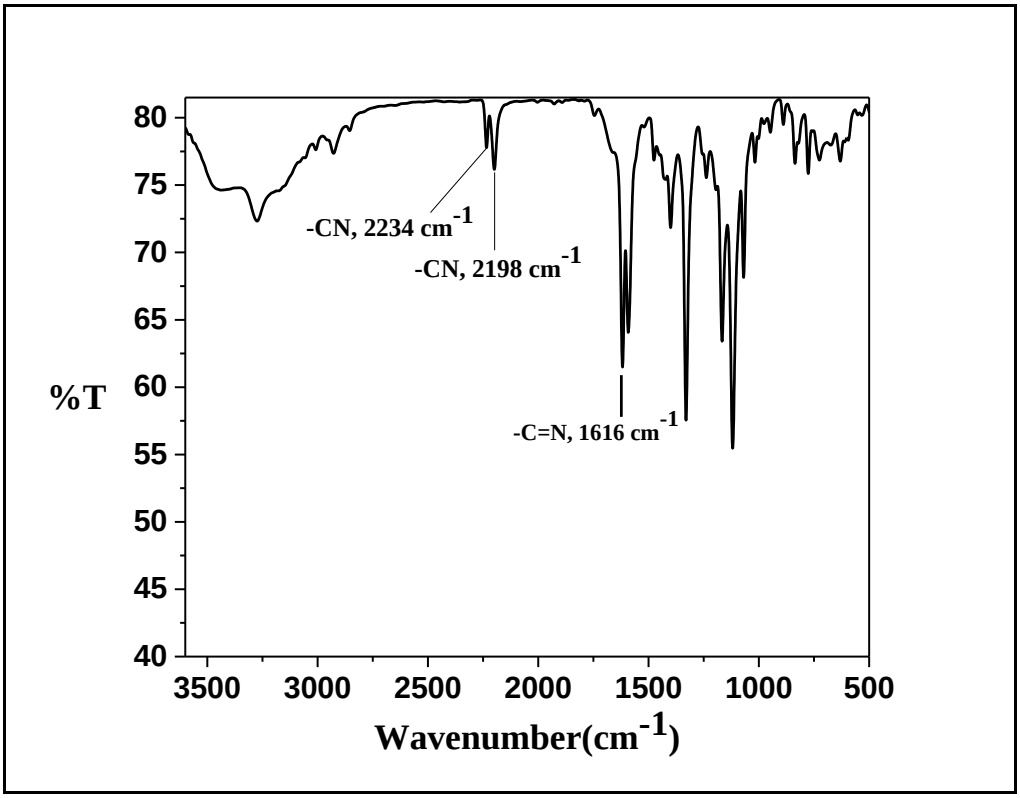


Figure S70: FTIR Spectrum of $Ni^{2\text{-}CF3}$.

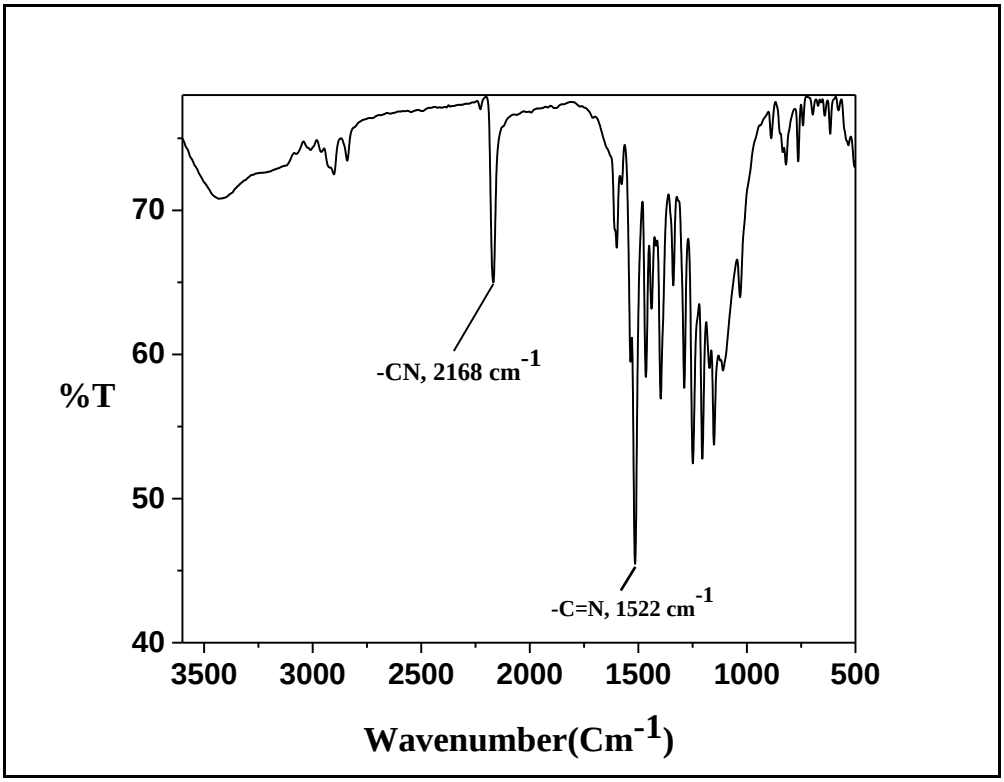


Figure S71: FTIR Spectrum of $Ni^{2\text{-}OMe}$.

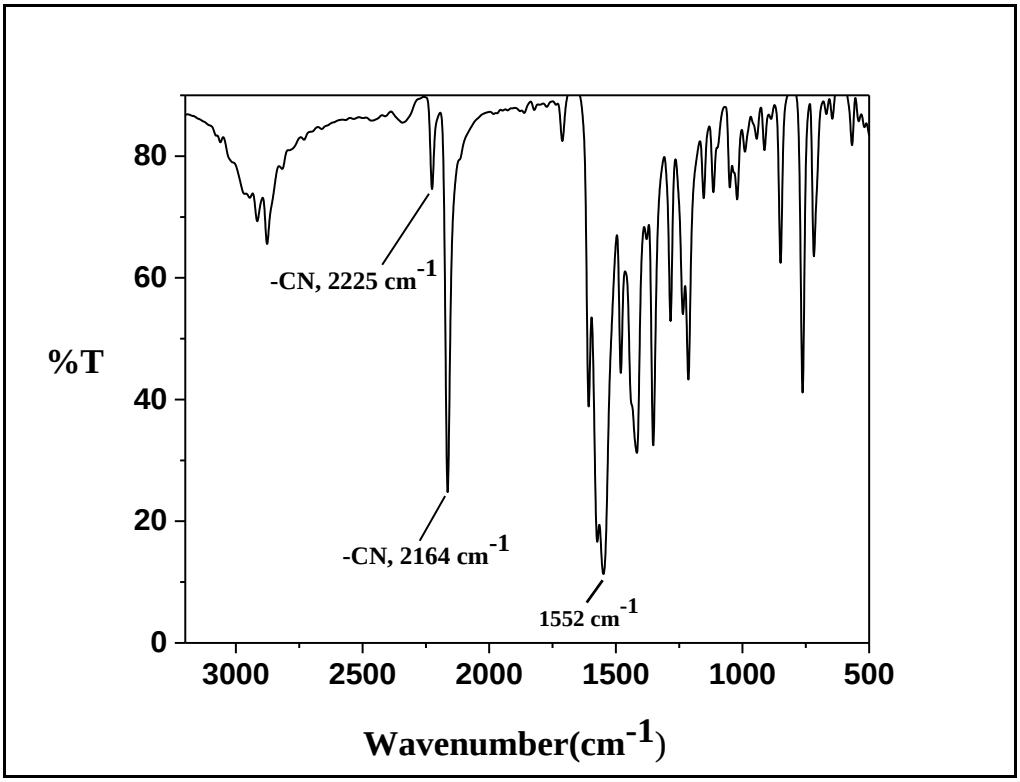


Figure S72: FTIR Spectrum of $\mathbf{Ni^{2\text{-}Mes}}$.

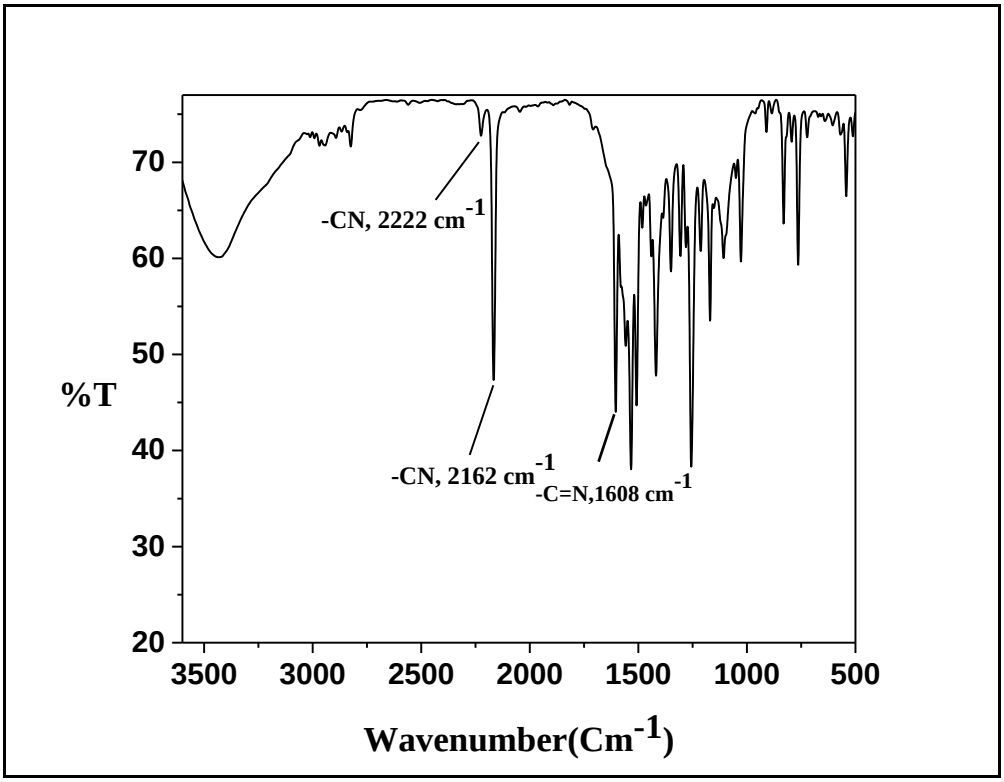


Figure S73: FTIR Spectrum of $\mathbf{Co^{1\text{-}CF3}}$.

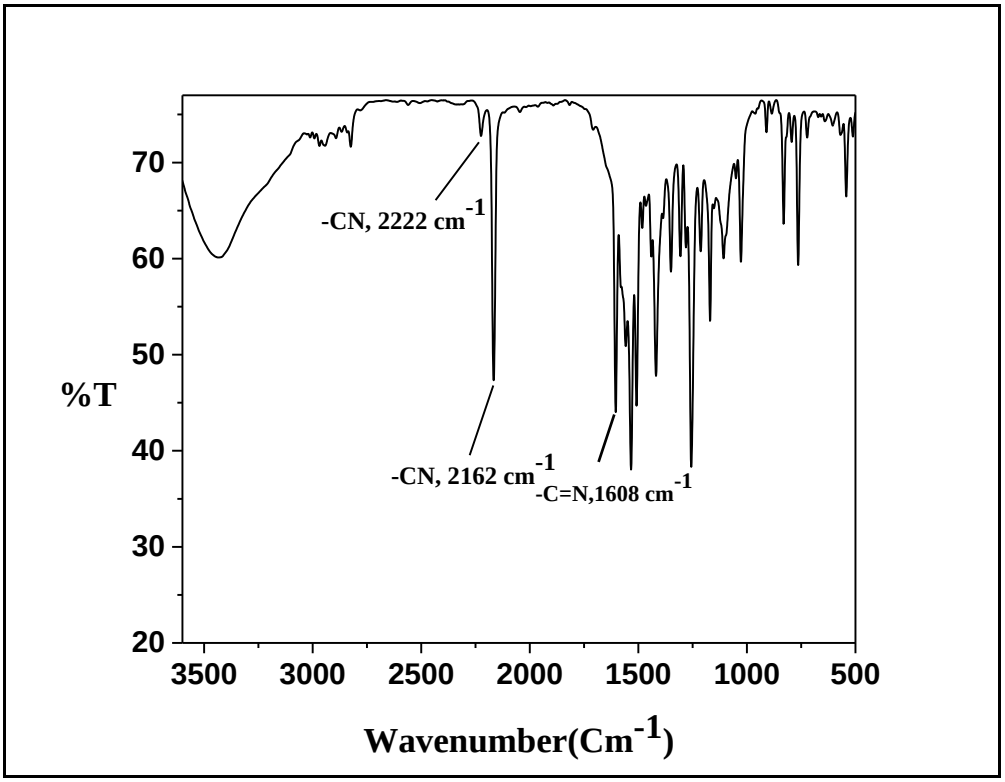


Figure S74: FTIR Spectrum of $\mathbf{Co^{1\text{-}OMe}}$.

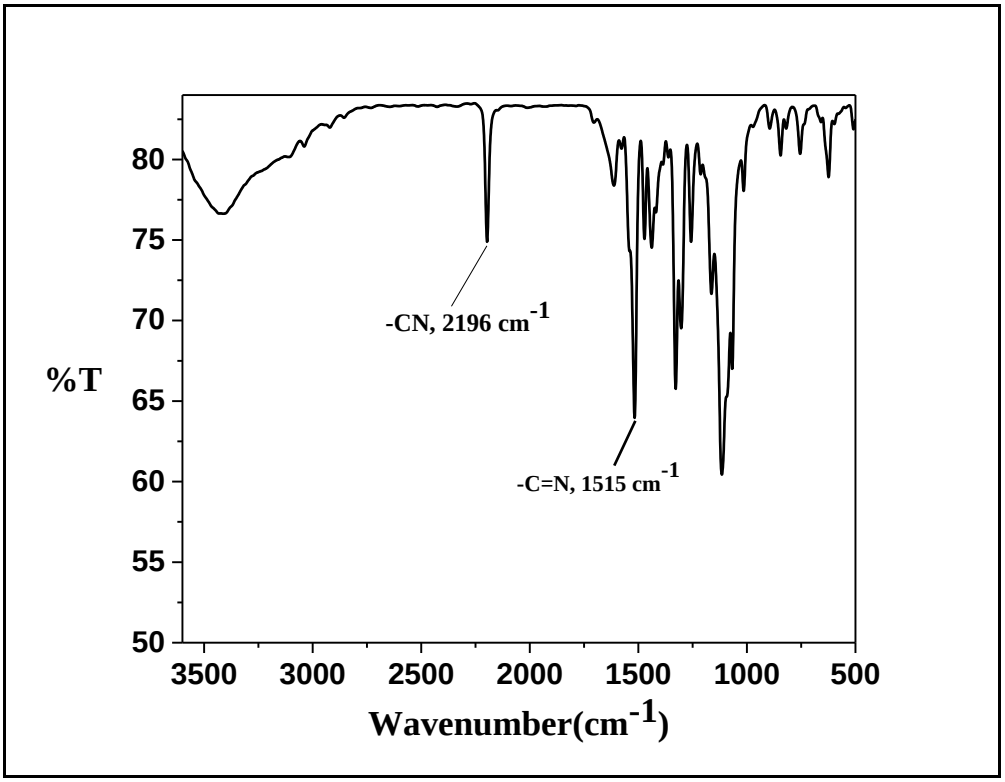


Figure S75: FTIR Spectrum of $\mathbf{Co^{2\text{-}CF3}.ClO_4}$.

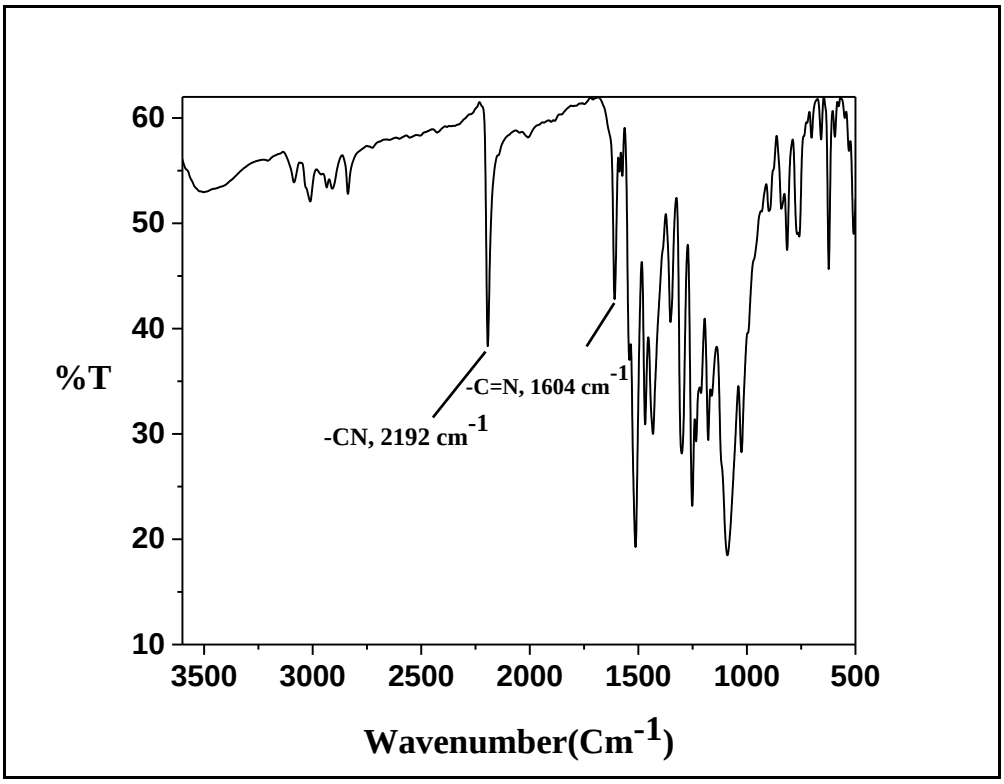


Figure S76: FTIR Spectrum of $\mathbf{Co^{2\text{-}OMe}.ClO_4}$.

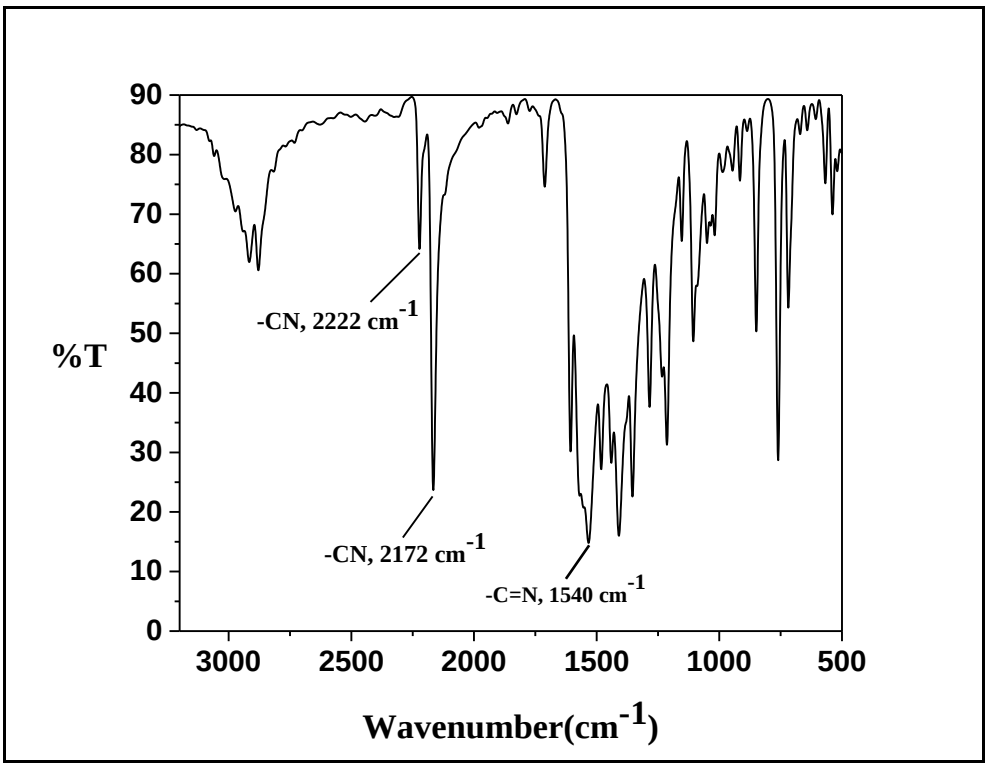


Figure S77: FTIR Spectrum of $\mathbf{Co^{2\text{-}Mes}}$.

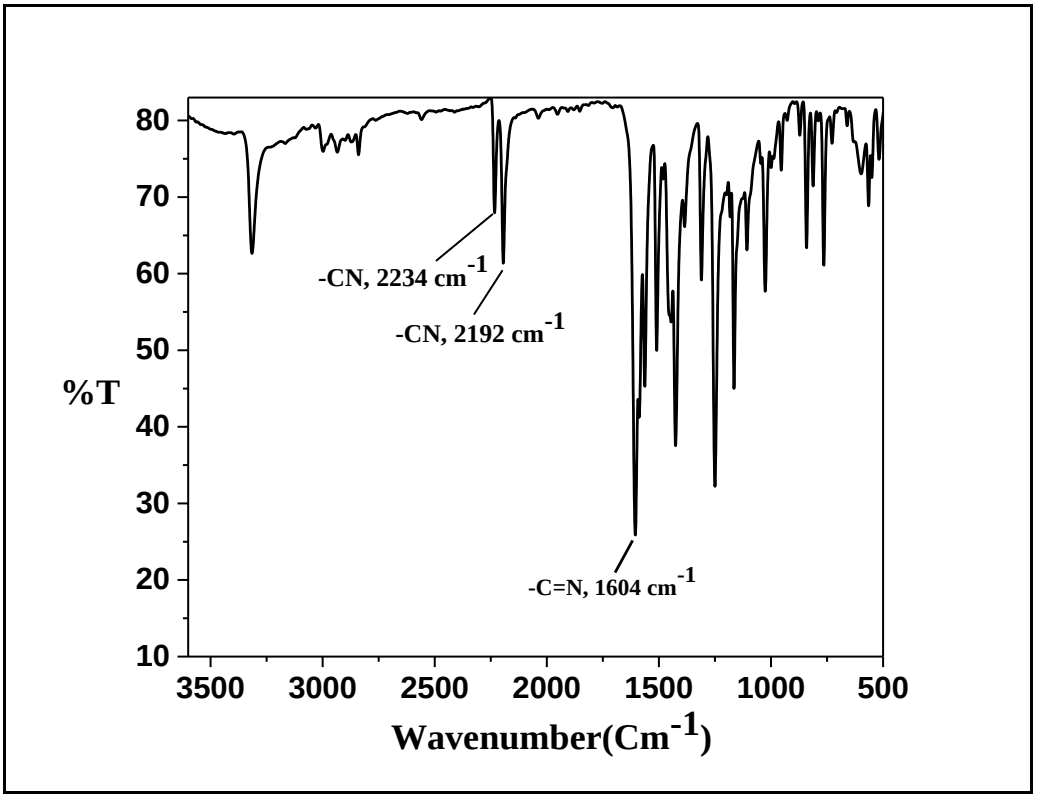


Figure S78: FTIR Spectrum of $\mathbf{C}^{\mathbf{OMe}}$.

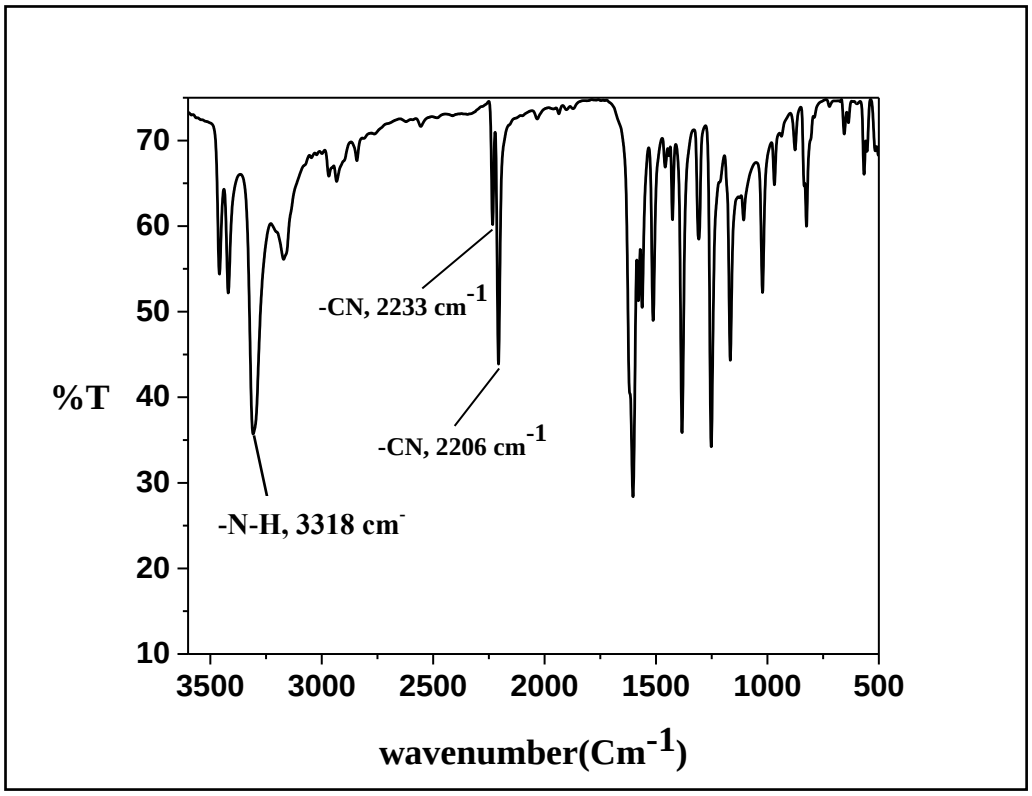


Figure S79: FTIR Spectrum of $\mathbf{D}^{\mathbf{OMe}}$.

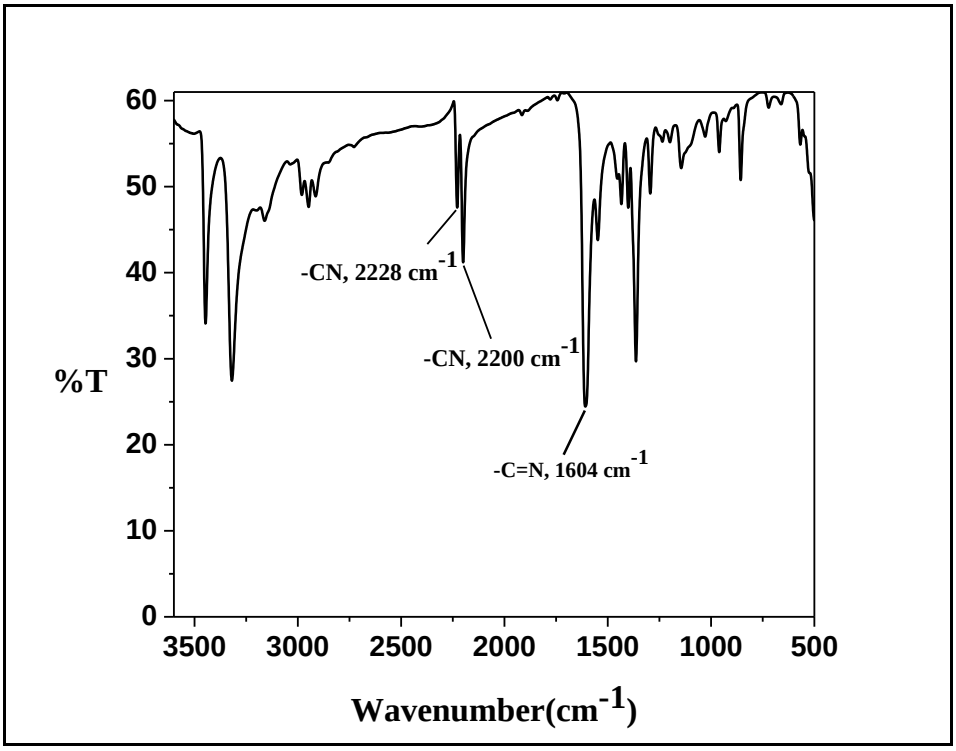


Figure S80: FTIR Spectrum of $\mathbf{C}^{\mathbf{Mes}}$.

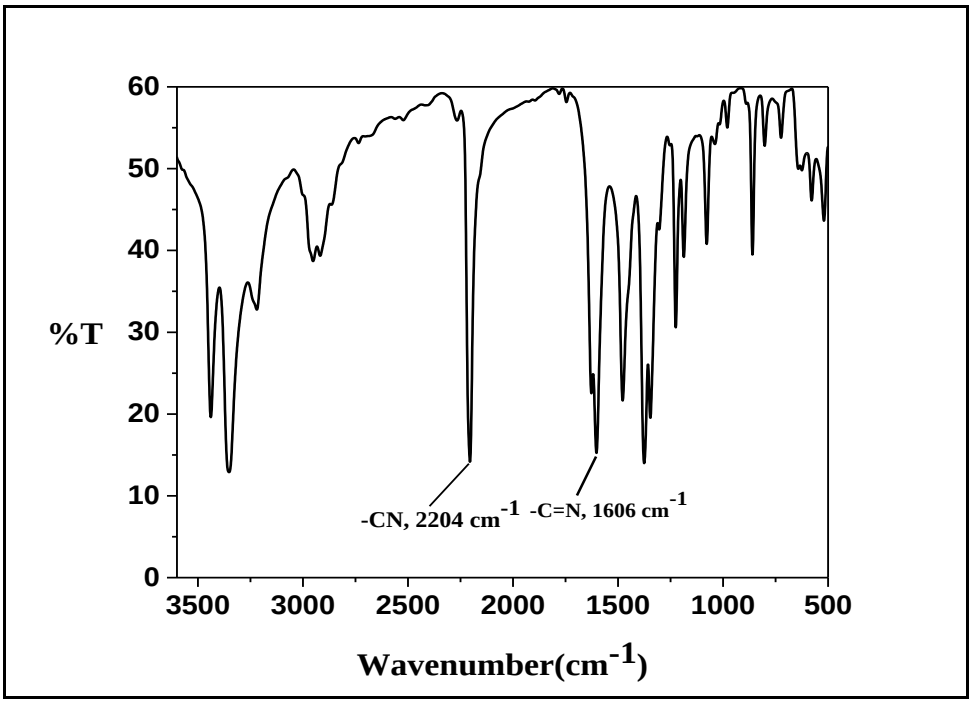


Figure S81: FTIR Spectrum of $\mathbf{D}^{\mathbf{Mes}}$.

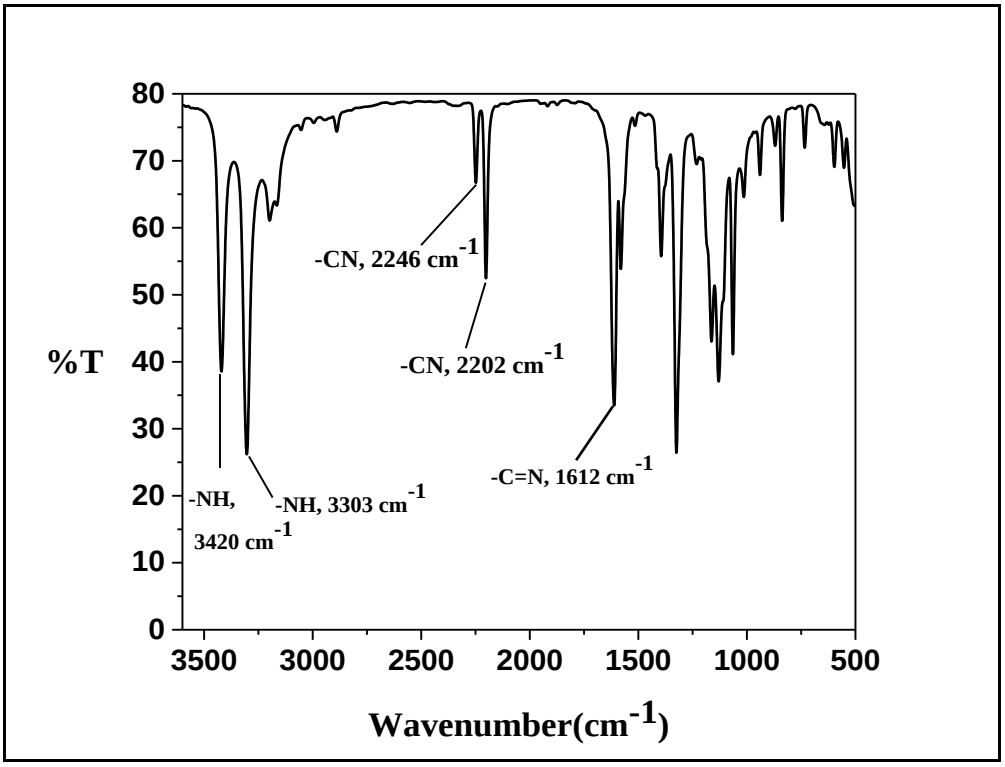


Figure S82: FTIR Spectrum of $\mathbf{C^{CF3}}$.

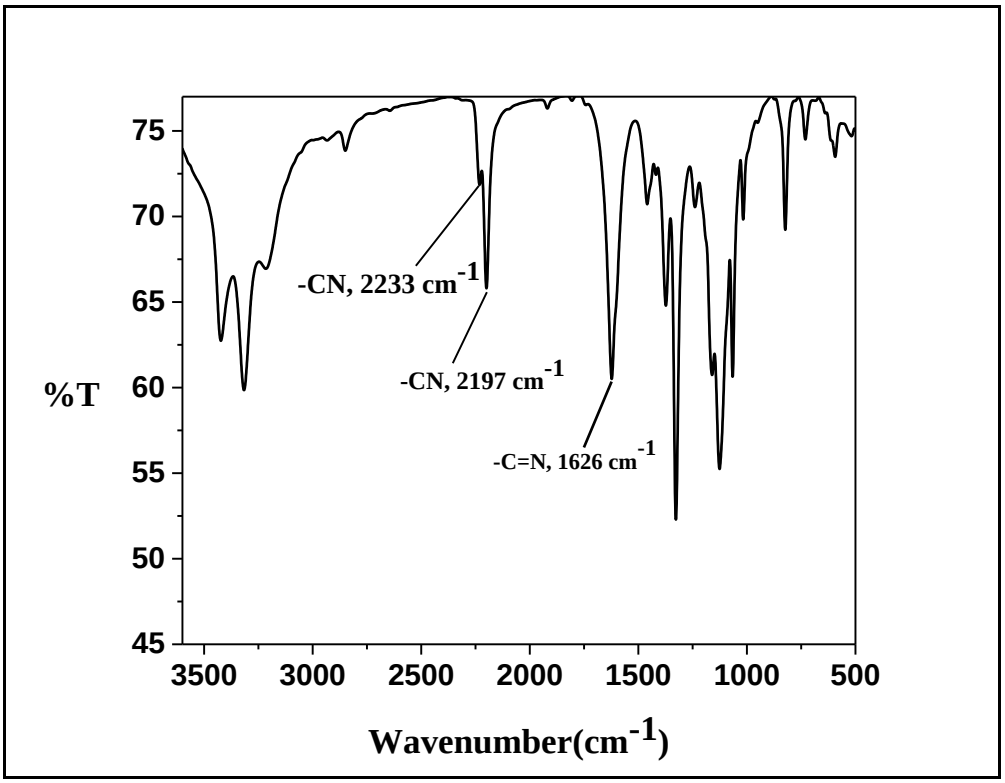


Figure S83: FTIR Spectrum of $\mathbf{D^{CF3}}$.

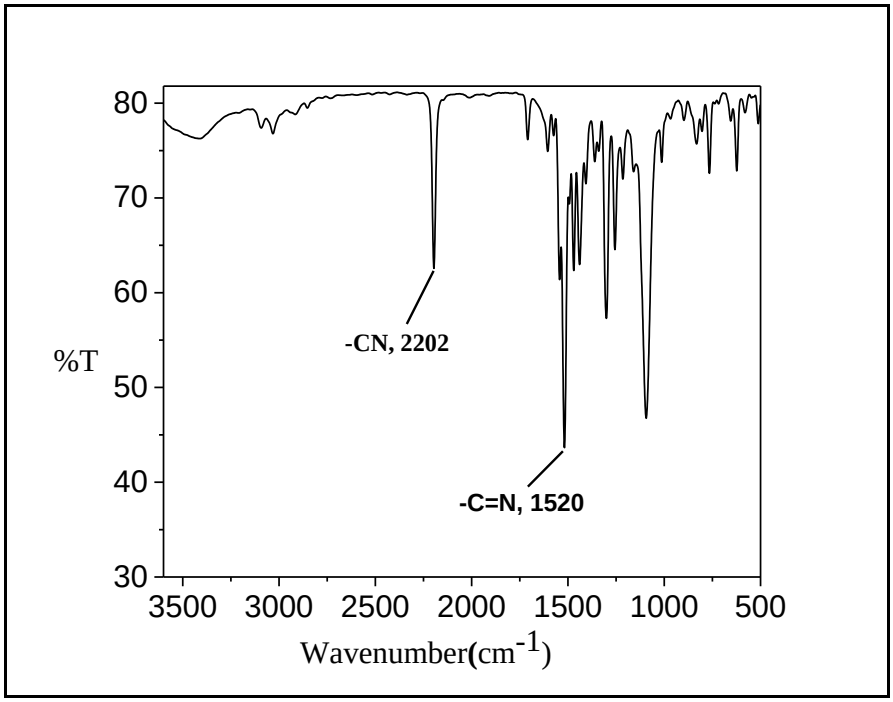


Figure S84: FTIR Spectrum of **Co**$^{2\text{-OMe}}$.

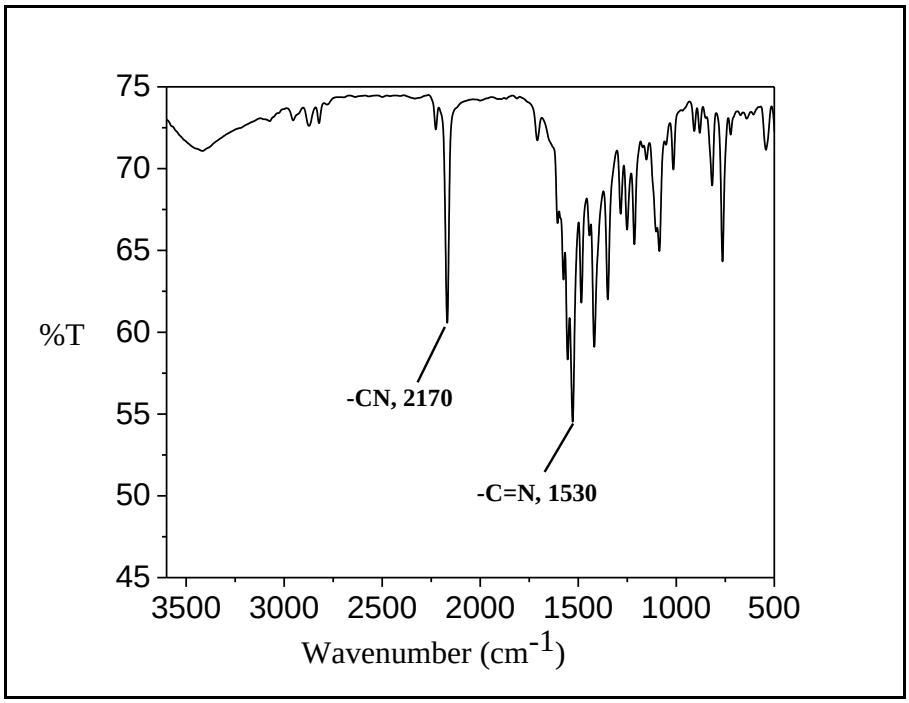


Figure S85: FTIR Spectrum of **Co**$^{2\text{-CF3}}$.

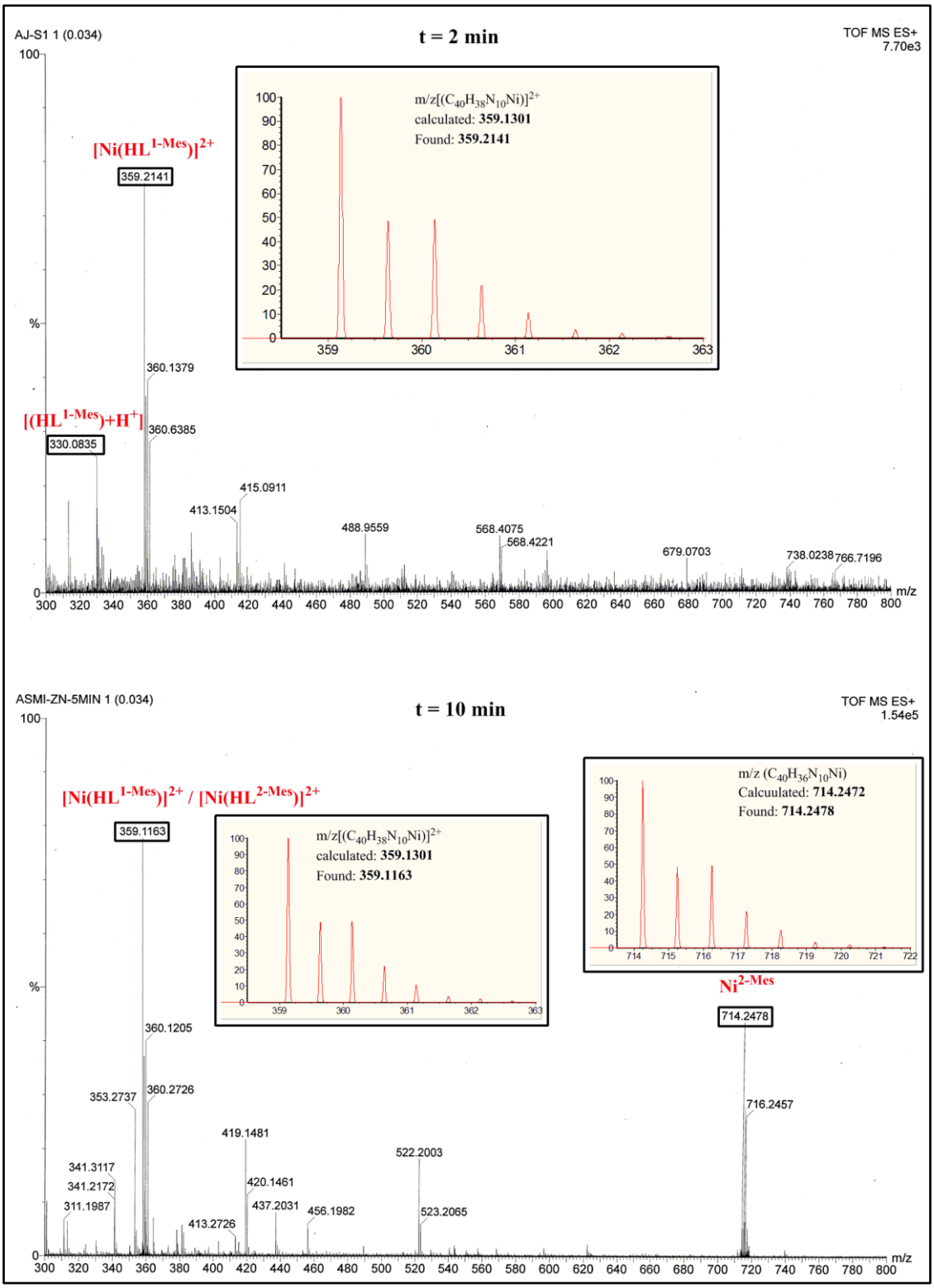


Figure S86: ESI-MS Spectrum of the reaction mixture of $Ni(ClO_4)_2$ with **HL$^{1\text{-Mes}}$** in acetonitrile at 2 minutes and at 10 minutes

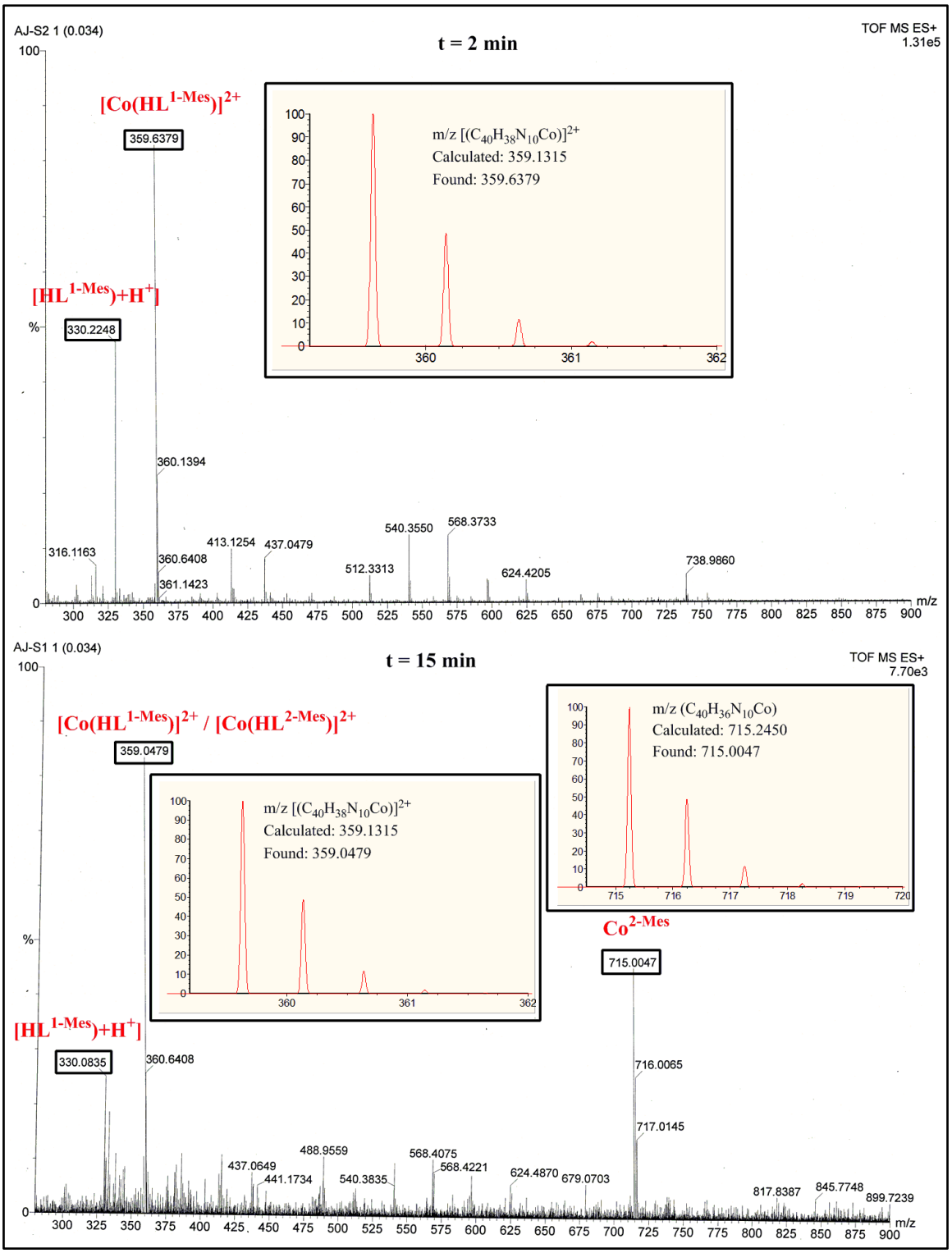


Figure S87: ESI-MS Spectrum of the reaction mixture of $Co(ClO_4)_2$ with **HL**$^{1\text{-Mes}}$ in acetonitrile at 2 minutes and at 15 minutes**.**

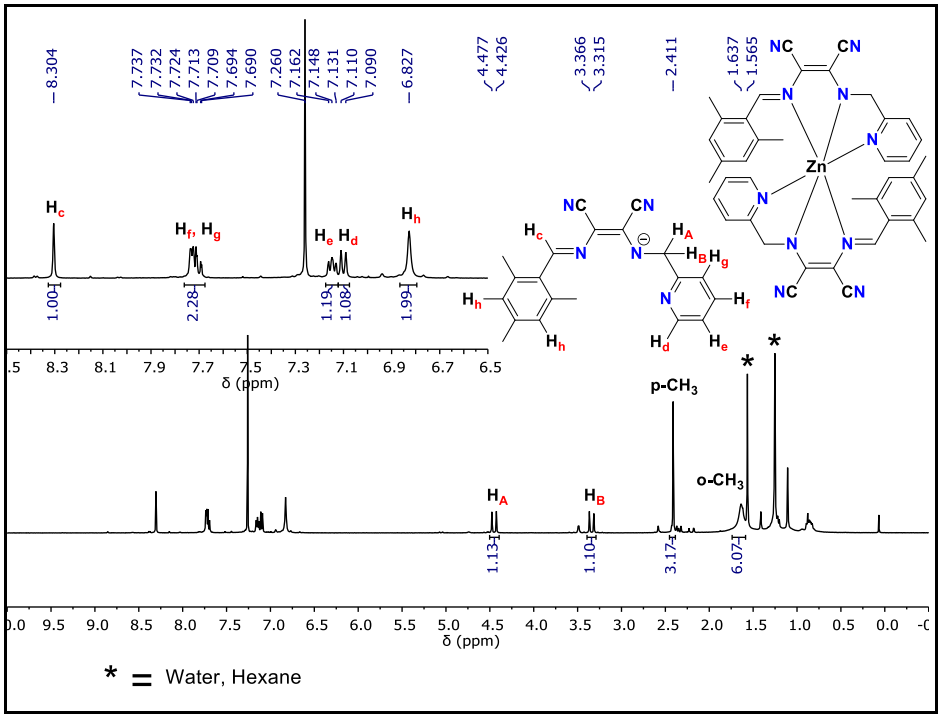


Figure S88: ^{1}H NMR Spectrum of **Zn$^{1\text{-Mes}}$** in $CDCl_3$.

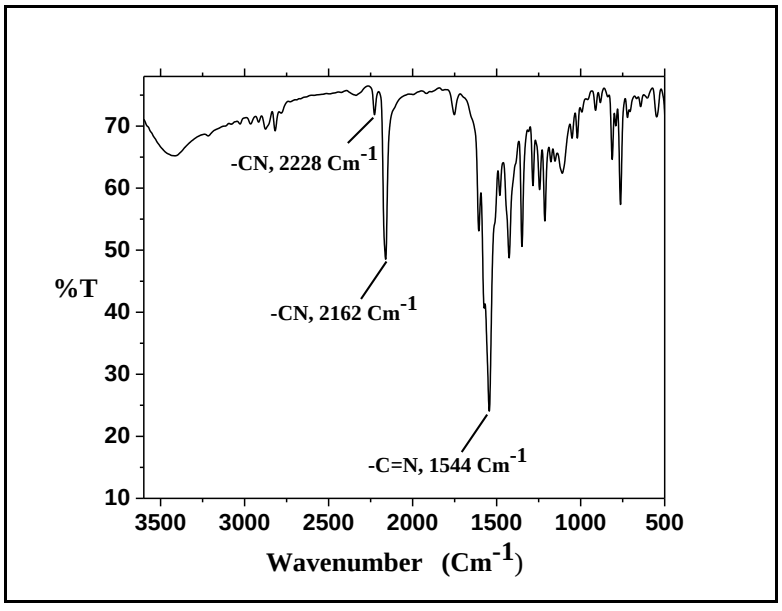


Figure S89: FTIR Spectrum of Zn$^{1\text{-Mes}}$.

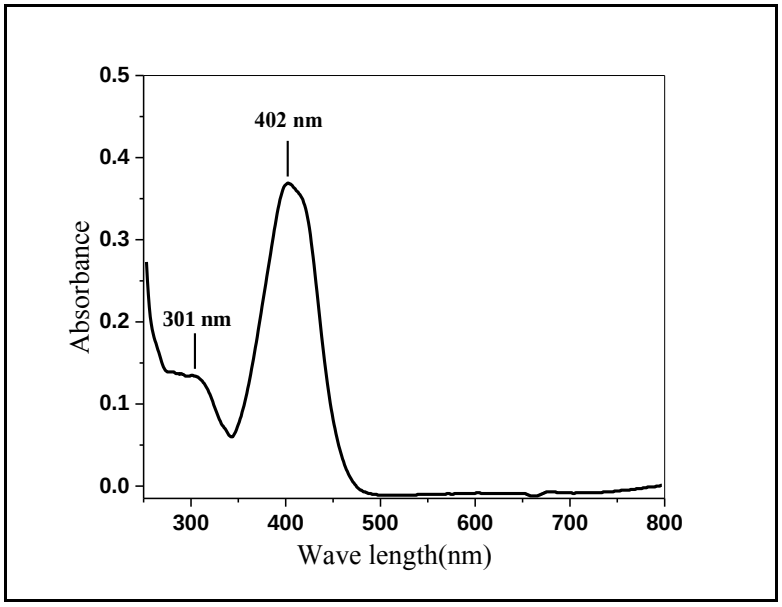
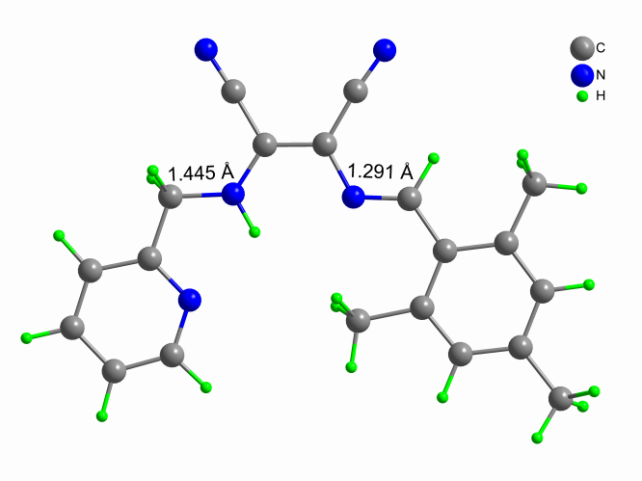


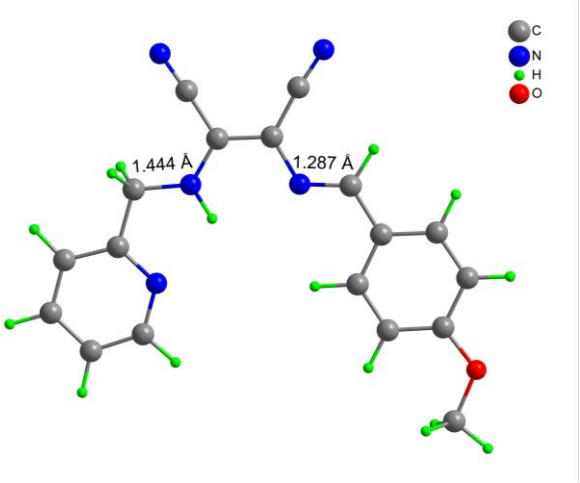
Figure S90: Electronic absorption spectra of $Zn^{1\text{-}Mes}$ (10^{-5} M) in acetonitrile.



Charge = 0, Multiplicity = 1

C	-0.23363300	2.22626100	-0.00107100	H	-6.11278100	-0.49088700	-0.00212100
C	-1.60667000	2.07871100	-0.00200300	C	-3.24654300	-2.98353000	0.00216100
C	-2.44912600	3.23769200	-0.00309700	C	-4.53879800	-3.48511600	0.00079500
C	0.34980400	3.52897300	-0.00168300	H	-6.62017200	-2.92734800	-0.00195400
N	-3.17237800	4.13536200	-0.00383600	H	-2.39338900	-3.65051400	0.00329800
N	0.92172100	4.53322900	-0.00199800	H	-4.71121900	-4.55155600	0.00085700
N	0.54423600	1.08007200	0.00001600	N	-2.96867200	-1.67481100	0.00215700
N	-2.21908800	0.87227300	-0.00249400	C	5.75766300	-3.08875200	-0.01300100
H	-1.63841300	0.04391000	-0.00016600	H	6.27863200	-3.11745200	-0.97266200
C	1.83277200	1.16741300	0.00082000	H	6.51278800	-2.92519200	0.75717400
H	2.29237500	2.15373100	0.00066000	H	5.31152300	-4.06812100	0.15214200
C	2.76619400	0.05066600	0.00141900	C	0.93655700	-1.76102200	0.00321100
C	4.15386300	0.36817100	0.00329500	H	0.39872300	-1.38690700	0.87359300
C	2.37324800	-1.31292500	0.00198200	H	0.39819500	-1.38926100	-0.86785600
C	5.08996000	-0.65646300	0.00428000	H	0.88758400	-2.84911000	0.00462900
C	3.35863500	-2.29760300	0.00286500	C	4.66237100	1.79324400	0.00616600
C	4.71733100	-2.00001300	0.00239700	H	4.33232200	2.35094900	-0.87126000
H	6.14235800	-0.40084300	0.00769400	H	4.32906100	2.34868000	0.88379500
H	3.04887800	-3.33527100	0.00522300	H	5.75040400	1.79961400	0.00811600
C	-3.64961800	0.66668700	0.00149100	C	-3.98242300	-0.81188700	0.00072500
H	-4.11229400	1.13442400	-0.87302300	C	-5.31660600	-1.22314900	-0.00084000
H	-4.10733000	1.13210100	0.87997000	C	-5.59631200	-2.57966200	-0.00074900

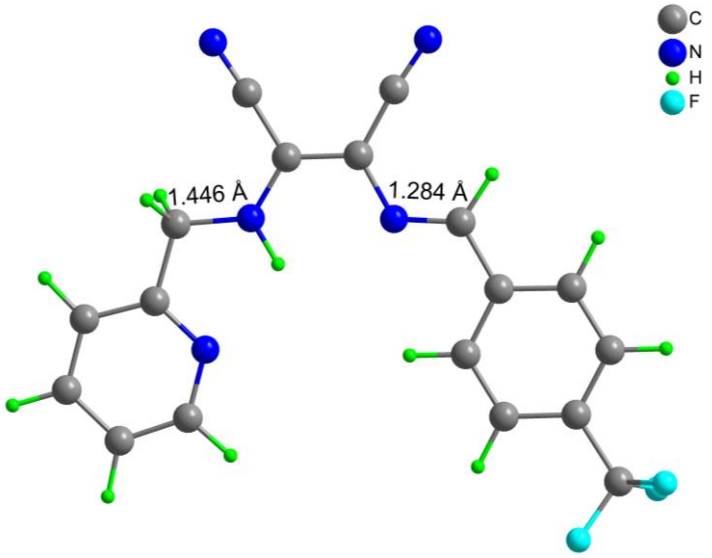
Figure S91: Geometry optimized molecular Structure of **HL**$^{\mathbf{1\text{-}Mes}}$**.**



Charge = 0, Multiplicity = 1

C	0.74811200	2.42853100	0.00010500	H	4.21957100	0.38285100	-0.87826400
C	2.04177100	1.94515800	0.00041900	C	3.58941400	-1.46117900	-0.00025200
C	3.14791600	2.85510300	0.00017200	C	4.77047500	-2.20591000	0.00007000
C	0.49515300	3.83214600	-0.00018400	C	4.68797600	-3.58831900	0.00020800
N	4.07348500	3.54233100	-0.00007500	H	5.72968800	-1.70592600	0.00022000
N	0.18184800	4.94451400	-0.00044900	C	2.31428600	-3.36685100	-0.00019500
N	-0.28350500	1.50608100	0.00014200	C	3.43131400	-4.18748900	0.00006900
N	2.32735200	0.62288300	0.00119100	H	5.58616100	-4.19034300	0.00045800
H	1.55047900	-0.02554000	0.00059700	H	1.31716100	-3.78946400	-0.00027100
C	-1.51563100	1.87683500	0.00012500	H	3.32043100	-5.26208100	0.00019000
H	-1.78594800	2.93599000	0.00014100	N	2.38583000	-2.03092600	-0.00036400
C	-2.62571300	0.93932700	0.00007800	O	-5.95004900	-1.56542500	-0.00006800
C	-3.94092300	1.43323700	0.00003000	C	-5.81750800	-2.98206300	-0.00006900
C	-2.44184700	-0.44867500	0.00007500	H	-6.83023500	-3.37314800	-0.00011600
C	-5.02642600	0.58010800	-0.00001900	H	-5.29396800	-3.33086000	-0.89236900
H	-4.10538400	2.50303100	0.00003200	H	-5.29404800	-3.33086800	0.89227500
C	-3.52221300	-1.31621600	0.00003000	H	-3.34660200	-2.38062700	0.00003300
H	-1.43584700	-0.84221100	0.00010800	C	3.65451800	0.05322600	-0.00071900
C	-4.82563600	-0.80413300	-0.00001900	H	4.22218600	0.38336400	0.87490000
H	-6.03853900	0.95801800	-0.00005800				

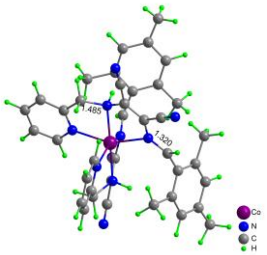
Figure S92: Geometry optimized molecular Structure of **HL$^{1\text{-OMe}}$.**



Charge = 0, Multiplicity = 1

C	1.59006700	2.44358900	0.00250800	H	4.83254000	0.04551900	0.90411300
C	2.82922900	1.82856200	0.01075700	H	4.84795200	0.06121900	-0.85015400
C	4.02166600	2.62475700	0.01586000	C	4.01204600	-1.71474300	0.00394300
C	1.47761800	3.86476000	-0.00281300	C	5.09993100	-2.58879300	0.00011900
N	5.00942900	3.21800100	0.02036700	C	4.85820500	-3.95285100	-0.01383300
N	1.27442000	5.00218400	-0.00781200	H	6.11038600	-2.20294200	0.00770700
N	0.47280000	1.62998600	-0.00057200	C	2.52532900	-3.46084600	-0.01861300
N	2.98240000	0.48981500	0.01423500	C	3.54138000	-4.40368600	-0.02353100
H	2.14724500	-0.08359900	0.00704800	H	5.68111100	-4.65416500	-0.01732700
C	-0.71613600	2.11501400	-0.01352200	H	1.48653800	-3.76636400	-0.02583900
H	-0.89147400	3.19323200	-0.02409700	H	3.30804700	-5.45833400	-0.03470000
C	-1.90599100	1.26876900	-0.01491100	N	2.75097300	-2.14216800	-0.00513600
C	-3.16872000	1.87562200	-0.04244700	C	-5.49369800	-1.09536400	0.00917400
C	-1.82930800	-0.13022900	0.00944400	F	-5.27327600	-2.39690600	-0.26440600
C	-4.32400700	1.11015800	-0.04645700	F	-6.40549900	-0.64937500	-0.88288400
H	-3.24080500	2.95487300	-0.06284500	F	-6.09215900	-1.04694600	1.22371300
C	-2.98167000	-0.89727200	0.00723000	H	-5.29210500	1.58917800	-0.07297600
H	-0.85884900	-0.60289500	0.02920700	H	-2.91557500	-1.97469400	0.02372600
C	-4.23165700	-0.27928900	-0.02203500	C	4.24458900	-0.21594400	0.01925200

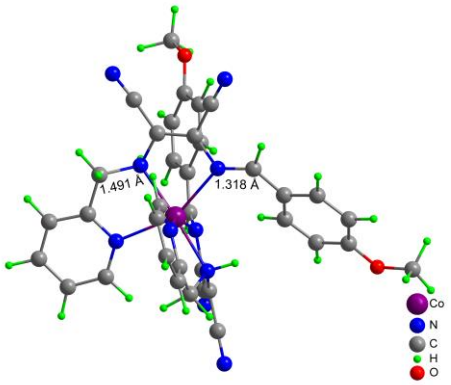
Figure S93: Geometry optimized molecular Structure of **HL**$^{\mathbf{1\text{-}CF3}}$**.**



Charge = 2, Multiplicity = 4

Co	2.11605942	-5.90824519	1.65146952	H	3.24733771	-3.47662355	-1.63499754
N	0.36589311	-6.60233243	0.59800154	H	5.04671863	-7.07775136	2.61086314
N	0.40151219	-4.84462343	2.77132424	H	5.27694313	-6.14284613	4.07463578
N	2.95822863	-7.46373488	0.26563074	H	3.66275285	-4.59910380	3.32148178
N	3.94653942	-5.29273193	2.62879356	H	-0.49470026	-4.13358563	4.49354805
N	2.90823944	-4.24640446	0.25298962	H	-0.14035098	-8.36366862	-0.51279653
N	2.22342068	-7.22863819	3.42815591	H	0.43328545	-8.63029168	1.12284803
C	0.58661328	-8.02909231	0.22605530	H	0.29912104	-6.05333881	-0.25952492
C	-0.82325885	-6.37631877	1.38570496	C	2.30673843	-4.96591288	5.69111772
C	-0.76682053	-5.53654230	2.45500123	H	1.48181617	-5.49243401	5.25847611
C	0.37085446	-4.06894377	3.83648555	H	3.22149036	-5.44763344	5.41530218
N	-2.93606997	-7.61296911	0.59306127	H	2.21067979	-4.96626056	6.75679713
C	-2.01813574	-7.03493166	0.98724017	C	0.21150848	-1.23903235	2.91134267
N	-2.87969873	-5.15505758	3.90001936	H	0.58072224	-1.12256413	1.91383760
C	-1.95845470	-5.33967581	3.23390624	H	-0.59533956	-1.94180732	2.91323093
C	4.22477477	-7.66527503	-0.13593941	H	-0.13688180	-0.29503408	3.27519906
C	1.99366876	-8.23125961	-0.27862534	C	4.18617317	-0.32649381	5.61385340
C	4.53262892	-6.45578127	3.34314002	H	3.73690694	0.27774023	6.37409092
C	4.81208337	-4.65523273	1.66771811	H	5.06631287	-0.79388689	6.00346579
C	4.27931417	-4.17024456	0.51203428	H	4.44886880	0.28831897	4.77845155
C	2.49368998	-3.76253168	-0.90357935	C	-2.73750989	-2.91627745	-2.80500887
N	7.29921162	-4.51460936	2.31258903	H	-2.69694829	-2.15257115	-3.55334533
C	6.19385747	-4.54494025	1.98172296	H	-3.16849185	-3.80219534	-3.22250623
N	5.82509177	-3.03834563	-1.22735924	H	-3.33694676	-2.58042798	-1.98477685
C	5.16050833	-3.53965180	-0.43134642	C	1.38428298	-5.74677546	-2.57417672
C	1.24591662	-7.97406726	3.97179340	H	2.34198842	-5.71312313	-2.09818531
C	3.43974265	-7.26075129	4.00292783	H	0.85996375	-6.62462153	-2.25893775
H	4.97938062	-7.02645717	0.29757625	H	1.51436877	-5.77102745	-3.63596273
C	4.58214880	-8.62483442	-1.06816964	C	1.04989800	-1.24734940	-0.19369169
H	5.61784278	-8.74162854	-1.35040779	H	0.31587242	-0.81449952	0.45341529
C	3.58404480	-9.41314553	-1.62655918	H	1.84892192	-1.65064335	0.39266551
H	3.82215723	-10.16859377	-2.36187596	H	1.43404525	-0.49528601	-0.85075450
C	2.27029943	-9.20601189	-1.22889460	H	2.87770467	-9.41300140	6.54995170
H	1.46628468	-9.79379775	-1.64843217	C	3.70497305	-8.02845604	5.13037325
C	1.34353490	-3.11060954	4.23345336	H	4.69180816	-8.01634292	5.57095447
C	2.31570350	-3.51429766	5.17698459	C	1.15628494	-3.53602204	-1.32476430
C	1.34279665	-1.75384084	3.82060572	C	0.57330426	-4.49686235	-2.18477879
C	3.27904331	-2.64672689	5.64358906	C	0.40346390	-2.37229727	-1.02327908
H	4.01106798	-2.99210325	6.35599352	C	-0.70288316	-4.34874184	-2.67990873
C	3.27779171	-1.31094987	5.20201439	H	-1.11733506	-5.10517890	-3.32684950
C	2.28223504	-0.87561758	4.29233408	C	-1.44107394	-3.19608327	-2.35236719
H	2.27045006	0.16974047	4.01906114	C	-0.85949181	-2.20415583	-1.52386876
H	0.27526851	-7.92003127	3.50096930	H	-1.43244671	-1.30856406	-1.33127404
C	1.43579585	-8.77747002	5.08280457	H	0.61452967	-9.35931047	5.47389992
				C	2.69215726	-8.80477025	5.67603442

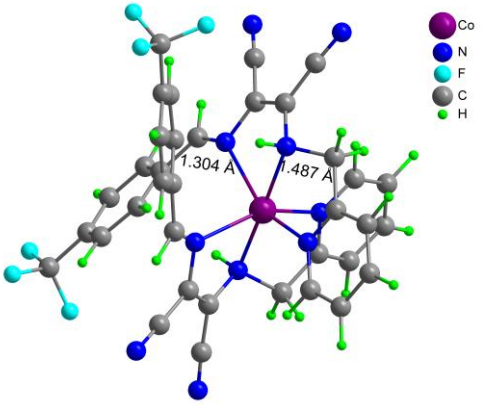
Figure S94: Geometry optimized molecular Structure of **$[Co(HL^{1\text{-}Mes})_2]^{2+}$.**



Charge = 2, Multiplicity = 4

Co	0.05599400	-0.91505800	0.07561900	C	4.38825200	3.22326100	1.24311500
N	-1.87851500	-0.99035600	1.02779500	H	5.23090700	3.63466500	1.77541600
N	0.23384000	0.71157400	1.70272600	C	4.30524300	3.31800500	-0.15810700
N	-0.89824300	-2.70800400	-0.88569400	C	3.16930800	2.79982700	-0.82841200
N	1.95769500	-0.94363200	-0.95752800	H	3.10574700	2.94177800	-1.89771100
N	-0.37743100	0.32453100	-1.82716100	H	1.27883700	1.85566100	-0.63846200
N	1.34674200	-2.13530100	1.40097000	H	0.23216900	-2.10470800	3.14321400
C	-2.31262800	-2.41571000	1.07895200	C	2.01300200	-3.26267400	3.41149800
C	-1.83489500	-0.34143100	2.31722700	H	1.78927000	-3.51086300	4.43829800
C	-0.77887600	0.45896100	2.62706700	C	3.17639000	-3.70622700	2.79432700
C	1.22819100	1.48200100	2.09629400	H	3.89029000	-4.31386900	3.33212100
N	-3.84525400	-0.79134000	3.85917300	C	3.41038300	-3.34701700	1.47431900
C	-2.92378100	-0.55613600	3.20520500	H	4.30912900	-3.66474300	0.96499800
N	-0.66748100	1.59452900	4.94998300	C	-2.50055500	1.55012900	-1.59575400
C	-0.74889600	1.08115800	3.92221700	C	-3.68176400	1.87337000	-2.30495500
C	-0.57803700	-3.34899000	-2.02262900	C	-2.39024400	1.99484900	-0.25338900
C	-2.00130800	-3.10923800	-0.22392100	H	-3.77298000	1.57660600	-3.34153000
C	2.66084600	-2.21527100	-0.64932600	C	-4.72275300	2.55112000	-1.71103200
C	1.74610700	-0.67617100	-2.35857500	H	-5.61087300	2.77368800	-2.28042300
C	0.59105500	-0.07215200	-2.75313500	C	-4.60164600	2.96600400	-0.37161600
C	-1.46941400	0.88643200	-2.31242000	C	-3.41047900	2.68554600	0.34324900
N	3.64731800	-1.38806000	-3.93973000	H	-3.32841600	3.06033500	1.35332500
C	2.77152500	-1.04288700	-3.27186600	H	-1.46652800	1.83868000	0.28239100
N	0.19310400	0.39860200	-5.26632800	H	-1.61363000	0.87026100	-3.39114200
C	0.40129800	0.18394600	-4.15403600	H	2.22871900	-2.99923900	-1.27063500
C	1.13555700	-2.47788500	2.68345100	H	3.71986400	-2.15789400	-0.89873900
C	2.47243600	-2.57003100	0.80544000	H	2.49434500	-0.17367700	-0.55671900
H	0.29793900	-2.99890100	-2.54756500	H	1.28905200	1.74213000	3.15162500
C	-1.31808000	-4.40111300	-2.53536400	H	-3.37206200	-2.49962100	1.31744500
H	-1.00994700	-4.87884800	-3.45339700	H	-1.76211600	-2.89840200	1.88711800
C	-2.45453700	-4.81061800	-1.84964100	H	-2.52491700	-0.47897100	0.42625200
H	-3.06170900	-5.62396900	-2.22098000	O	-5.52178400	3.63786100	0.30079500
C	-2.80253400	-4.14812200	-0.68046800	O	5.21039500	3.89028600	-0.93609800
H	-3.68489900	-4.43279500	-0.12518700	C	6.38787400	4.49882300	-0.36402200
C	2.24758100	2.05473100	1.28702300	H	6.98704200	3.75245000	0.15507900
C	3.36590700	2.61926400	1.94198600	H	6.93988700	4.89502400	-1.20795700
C	2.16974000	2.18352100	-0.12316100	H	6.10673100	5.30671100	0.30933000
H	3.42615300	2.57005700	3.02127700	C	-6.76314400	4.01486400	-0.33291600
H	-6.57086900	4.67089500	-1.18014000	H	-7.31372800	3.12905800	-0.64520300
				H	-7.31930700	4.54725400	0.42939200

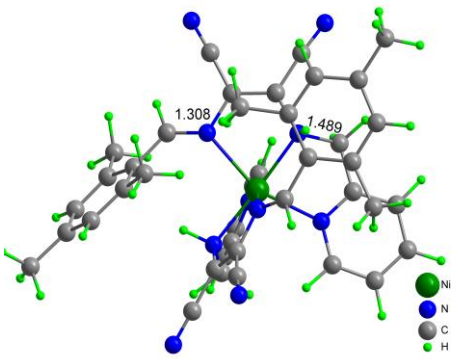
Figure S95: Geometry optimized molecular Structure of **$[Co(HL^{1\text{-}OMe})_2]^{2+}$.**



Charge = 2, Multiplicity = 4

Co	-0.05431600	1.22056600	0.07978700	H	-0.66125700	3.24089800	-2.47441300
N	1.97579200	1.25515000	0.80284100	C	0.97025900	4.59455100	-2.74992000
N	-0.04054200	-0.41301700	1.78189400	H	0.52827800	5.06940900	-3.61317100
N	0.78483900	2.93485100	-1.02505100	C	2.21428900	4.98077000	-2.26645300
N	-2.05253800	1.14410400	-0.76411800	H	2.77368800	5.77087700	-2.74707100
N	0.17033100	-0.13183000	-1.87588800	C	2.73028600	4.32797300	-1.15517800
N	-1.22328700	2.41290200	1.48606100	H	3.69658000	4.59894700	-0.75397200
F	-5.24199700	-4.30354900	-1.23556100	C	-2.09883800	-1.74044200	1.60865900
C	-5.58099500	-3.45690300	-0.25231100	C	-3.18078600	-2.16985900	2.39514000
F	-6.29807400	-2.45588800	-0.80382200	C	-2.14256600	-1.94296900	0.21593300
F	-6.36802400	-4.10306600	0.61127000	H	-3.13980300	-2.06755400	3.47117200
F	6.66066900	-3.64371300	-1.05226500	C	-4.30948800	-2.71807300	1.80278100
C	5.82272300	-3.17230900	-0.12553100	H	-5.14399400	-3.03387700	2.41080500
F	6.47956300	-2.24552400	0.60062100	C	-4.34846300	-2.88617100	0.42319900
F	5.49239500	-4.17709700	0.69967100	C	-3.25586900	-2.51793700	-0.36870000
C	2.48429300	2.65555700	0.70736500	H	-3.27693500	-2.71545400	-1.43096400
C	2.07354200	0.67602300	2.12061900	H	-1.27552100	-1.71425200	-0.38616900
C	1.07683800	-0.12080100	2.58358200	H	0.12066500	2.51115500	3.05715500
C	-0.94933400	-1.19357100	2.29402100	C	-1.66353500	3.59545800	3.52711700
N	4.20326500	1.25264400	3.44758100	H	-1.31407500	3.89853700	4.50283900
C	3.23707900	0.96139100	2.88853000	C	-2.92237900	3.95701800	3.06205900
N	1.21485800	-1.15665200	4.94802300	H	-3.58695800	4.55265600	3.67175900
C	1.18927000	-0.68515700	3.89735900	C	-3.31515800	3.53370500	1.79986200
C	0.29813400	3.57067700	-2.10584500	H	-4.28947500	3.79054400	1.40869400
C	1.98849800	3.31885900	-0.55439300	C	2.31871500	-1.33088300	-1.81842200
C	-2.80245300	2.36769100	-0.37296700	C	3.44659400	-1.57735700	-2.62126900
C	-1.99454000	0.87396100	-2.17685400	C	2.33196300	-1.74898600	-0.47417800
C	-0.90345200	0.25576500	-2.69944400	H	3.43346000	-1.30287700	-3.66745200
C	1.16975700	-0.73413100	-2.45887100	C	4.58138900	-2.16525500	-2.08258800
N	-4.02405400	1.63553900	-3.56614200	H	5.44841400	-2.34331900	-2.70093900
C	-3.10041700	1.26625900	-2.98175800	C	4.58584400	-2.55074900	-0.74654700
N	-0.77236000	-0.24070100	-5.23279400	C	3.45442500	-2.35887200	0.05311300
C	-0.86630600	-0.01252500	-4.10757300	H	3.45636100	-2.71753800	1.07240500
C	-0.85515900	2.82137200	2.71386500	H	1.43974100	-1.64988200	0.12477300
C	-2.43895400	2.77431400	1.03449000	H	1.16513800	-0.82294200	-3.54443000
H	-2.52685300	3.16826700	-1.05923200	H	3.57163000	2.68572100	0.75833900
H	-3.87797300	2.22344400	-0.46871100	H	2.10793800	3.20267300	1.57249000
H	-2.48020000	0.34000500	-0.30150300	H	2.50927800	0.67143400	0.15680700
H	-0.85773500	-1.49391900	3.33708600				

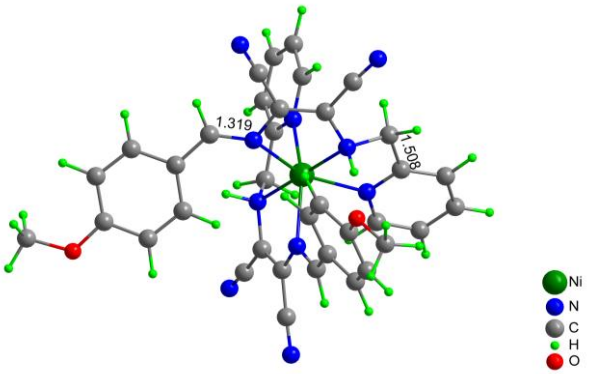
Figure S96: Geometry optimized molecular Structure of **$[Co(HL^{1\text{-}CF3})_2]^{2+}$.**



Charge = 2, Multiplicity = 3

Ni	0.00000000	0.00000000	0.00000000	C	-1.07036897	3.20700793	1.87791245
N	0.00000000	0.00000000	2.09371924	C	-2.26720154	3.46094661	2.60783022
N	2.25791417	0.00000000	0.42515950	C	0.18668525	3.24630855	2.54891666
N	-2.09581576	-0.36838980	0.42708422	C	-2.19172390	3.61981511	3.98497832
N	0.08121768	0.10906613	-2.08932734	H	-3.10557856	3.78002500	4.54127474
N	-0.62064929	2.18637630	-0.33604451	C	-0.97569776	3.60141847	4.67007571
N	0.25517638	-2.08978813	-0.52700640	C	0.19723109	3.43203722	3.92374501
C	-1.08384470	-0.89610140	2.58210188	H	1.15083474	3.49114050	4.43220983
C	1.31098562	-0.28152974	2.62399709	H	-1.93987281	3.72143018	-0.00969258
C	2.38766796	-0.28297468	1.79647657	H	-1.54026409	-1.09347613	-2.67300496
C	3.28454772	-0.28645195	-0.33326703	H	-0.13335762	-1.28560078	-3.69922273
N	1.40097326	-0.70451435	5.16159948	H	1.08150349	0.15408091	-2.30427878
C	1.41708240	-0.51796559	4.02316274	H	4.11460434	-0.81742371	0.12899965
N	4.74330792	-0.78016786	2.74073022	H	-1.33881152	-0.68058345	3.61928652
C	3.68325071	-0.55710997	2.34907345	H	-0.71732470	-1.92173120	2.55030457
C	-3.15916387	-0.26230418	-0.38660554	H	-0.24795231	0.96020159	2.34931523
C	-2.30003151	-0.76448760	1.69640284	C	4.48578976	-2.37573878	-1.88211778
C	-0.45244823	-1.15559982	-2.66554351	H	3.65665124	-2.90176563	-1.40758568
C	-0.53862332	1.31423770	-2.58177877	H	4.90990297	-3.03681049	-2.63319902
C	-0.87599284	2.30274004	-1.71397815	H	5.25379283	-2.22247065	-1.12023110
C	-1.21413239	3.05060853	0.44630056	C	2.77935044	2.44654195	-1.57756850
N	-0.87205232	1.41395286	-5.13233293	H	1.90027131	2.30800928	-0.95712878
C	-0.74147415	1.42243618	-3.98604528	H	3.59697368	2.73256534	-0.91319015
N	-1.98170822	4.47028701	-2.58975126	H	2.59724463	3.28482310	-2.24578419
C	-1.48348497	3.49642314	-2.22887207	C	4.16003867	0.50990693	-5.97669344
C	0.62555661	-3.12160013	0.24904327	H	5.05394062	1.12045961	-6.12557087
C	-0.01737396	-2.33051475	-1.82220221	H	4.31720178	-0.43551030	-6.49055491
H	-2.96898003	0.08798277	-1.39070528	H	3.33276610	1.03541713	-6.45300726
C	-4.44888674	-0.56671570	0.01300583	C	-0.91218186	3.82005128	6.15295404
H	-5.26716198	-0.46990872	-0.68496160	H	-0.56981976	4.83509674	6.36825418
C	-4.65687782	-0.98586575	1.32219296	H	-1.88505614	3.69323828	6.62189224
H	-5.64981396	-1.22941155	1.67286048	H	-0.20380737	3.13898816	6.62410184
C	-3.56721898	-1.07407885	2.17694980	C	-3.61507729	3.53406962	1.93235962
H	-3.69380275	-1.37916998	3.20611631	H	-3.86641080	2.61630494	1.39954635
C	3.44999490	-0.03156262	-1.74826188	H	-4.39718160	3.71572166	2.66470435
C	4.06056336	-1.07007734	-2.50888562	H	-3.65669842	4.35266674	1.20988759
C	3.15818998	1.21837285	-2.36823325	C	1.50085021	3.26896569	1.80760563
C	4.24512631	-0.88294552	-3.87206297	H	2.33044299	3.29707730	2.51000906
H	4.67885939	-1.68545454	-4.45355819	H	1.64097161	2.41862685	1.14863014
C	3.91002469	0.31222167	-4.51069115	H	1.56815716	4.16621452	1.18945818
C	3.38672401	1.35068502	-3.73027845	H	1.01034232	-5.21581695	0.45383665
H	3.19316304	2.30704129	-4.19857111	C	0.42149191	-4.67107920	-1.55211696
H	0.86851110	-2.89339904	1.27665936	H	0.48210910	-5.67283574	-1.95338163
C	0.71358626	-4.42233048	-0.21580463	C	0.06245239	-3.60689699	-2.36719511
				H	-0.15420102	-3.76020707	-3.41497642

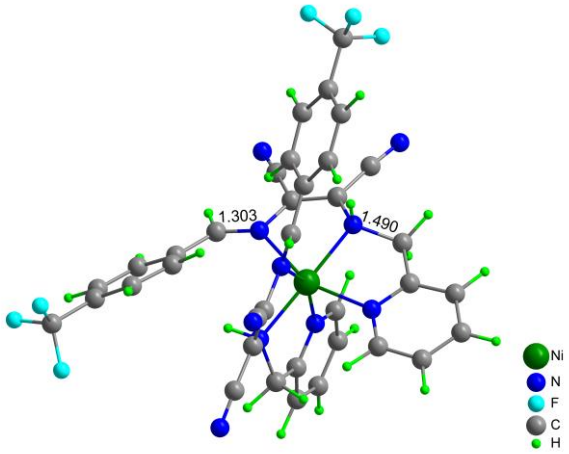
Figure S97: Geometry optimized molecular Structure of **$[Ni(HL^{1\text{-}Mes})_2]^{2+}$.**



Charge = 2, Multiplicity = 3

Ni	0.00000000	0.00000000	0.00000000	H	2.50285062	3.03550234	-3.67036054
N	0.00000000	0.00000000	2.10794739	H	1.94024686	2.00858570	-1.49299534
N	2.23986734	0.00000000	0.44697590	H	0.81354919	-2.86816845	1.41934401
N	-2.13574041	-0.16770043	0.43521128	C	0.65986271	-4.45595538	-0.00559266
N	-0.02405971	-0.02827827	-2.10762013	H	0.97388759	-5.21538415	0.69485070
N	-0.36708773	2.20427406	-0.47244679	C	0.35609947	-4.76602994	-1.32516760
N	0.17472105	-2.14044468	-0.40854764	H	0.42676297	-5.78267038	-1.68504709
C	-1.17574270	-0.77204724	2.59116144	C	-0.03133288	-3.74184201	-2.17777349
C	1.27614639	-0.46503856	2.59692086	H	-0.26504215	-3.94224257	-3.21375806
C	2.34562713	-0.47350356	1.75482822	C	-0.00400862	3.60761766	1.51395796
C	3.32576760	-0.05700721	-0.29916967	C	-0.57515265	4.67696729	2.24279328
N	1.33299789	-1.19882493	5.06224245	C	1.17453980	3.00855097	2.02826845
C	1.36008643	-0.87550896	3.95456305	H	-1.45040352	5.17671213	1.84893923
N	4.63660476	-1.32562722	2.60462788	C	-0.05172932	5.09650451	3.44556579
C	3.60681236	-0.94507199	2.25645858	H	-0.51850220	5.90952400	3.97812636
C	-3.19136347	0.04320211	-0.36896430	C	1.10412114	4.47275101	3.95134798
C	-2.37421126	-0.48990874	1.72046725	C	1.71635271	3.42940577	3.21333286
C	-0.60136912	-1.31963635	-2.56699960	H	2.63352195	3.00893015	3.59993197
C	-0.69482830	1.14934060	-2.60480543	H	1.68583453	2.25883845	1.44325775
C	-0.86643382	2.21461656	-1.77491678	H	-1.28137874	4.02441966	-0.12294614
C	-0.59016331	3.27665806	0.26198921	H	-1.68624352	-1.24666671	-2.49733844
N	-1.45625470	1.05388392	-5.06053402	H	-0.36075052	-1.51381635	-3.61150941
C	-1.12893616	1.14767929	-3.95768073	H	0.95403274	0.00901509	-2.39606084
N	-2.08720382	4.32634609	-2.63931477	H	4.17969710	-0.61319884	0.08366104
C	-1.54129188	3.37627786	-2.28453554	H	-1.39434131	-0.55195510	3.63537303
C	0.56259997	-3.13728328	0.40470774	H	-0.92918318	-1.83173664	2.53288915
C	-0.11933896	-2.44503217	-1.68656395	H	-0.11801680	0.97505736	2.38468802
H	-2.97792685	0.32067470	-1.38991468	O	1.70964387	4.79873833	5.08175267
C	-4.50365748	-0.06821367	0.05785678	C	1.20492159	5.87648538	5.89917351
H	-5.31178596	0.10965829	-0.63586773	H	0.19600755	5.65271483	6.24179078
C	-4.74550229	-0.40032431	1.38484939	H	1.87993452	5.92971189	6.74498947
H	-5.75602915	-0.48989886	1.75750961	H	1.22754787	6.81335587	5.34515450
C	-3.66251290	-0.60584739	2.22799746	O	4.40147025	2.39254749	-5.16522672
H	-3.81068755	-0.85492043	3.26917529	C	5.53725657	2.05731849	-5.99110185
C	3.54342785	0.55779679	-1.56217484	H	5.47554852	1.02095120	-6.31897661
C	4.68265004	0.15686931	-2.29861449	H	5.47113917	2.72050895	-6.84531834
C	2.75602625	1.61709692	-2.08203287	H	6.46438741	2.23838565	-5.44997369
H	5.32166944	-0.62081296	-1.90138162	C	4.19043983	1.75777869	-4.02361712
C	4.99843329	0.72473773	-3.51288396	C	3.07033830	2.20356508	-3.27882917
H	5.87008035	0.38810333	-4.05084925				

Figure S98: Geometry optimized molecular Structure of **$[Ni(HL^{1\text{-}OMe})_2]^{2+}$.**



Charge = 2, Multiplicity = 3

Ni	0.00000000	0.00000000	0.00000000	C	2.83195512	1.62361646	-2.02027926
N	0.00000000	0.00000000	2.10917680	H	5.23507219	-0.78999532	-1.91393982
N	2.27359267	0.00000000	0.49138882	C	4.89076183	0.52801130	-3.56251732
N	-2.11780103	-0.15876063	0.41384165	H	5.69444424	0.12113652	-4.15786102
N	0.02293749	0.02675506	-2.10880258	C	4.13367255	1.59037192	-4.04530340
N	-0.36246853	2.24963536	-0.46675887	C	3.11757011	2.15173063	-3.26595798
N	0.19069239	-2.11032838	-0.43869714	H	2.58181216	3.01602513	-3.63125573
F	4.25491586	3.48123037	-5.45027426	H	2.08900147	2.09180440	-1.39202370
C	4.38682892	2.14687593	-5.43398958	H	0.74958631	-2.86284859	1.40707897
F	3.48566816	1.63518644	-6.29678175	C	0.64613661	-4.43287309	-0.03997371
F	5.60779017	1.83614624	-5.87745362	H	0.92730241	-5.20127160	0.66470010
F	0.84095529	5.75541835	5.96062180	C	0.39376401	-4.72792579	-1.37402544
C	1.34971595	4.60635808	5.50809028	H	0.47377163	-5.74116029	-1.74156096
F	0.98091093	3.62353850	6.35449241	C	0.04425628	-3.69321820	-2.23043116
F	2.68758460	4.69137668	5.54013057	H	-0.15062912	-3.88286958	-3.27653593
C	-1.19810571	-0.73771127	2.59807991	C	-0.07020742	3.59012438	1.57347871
C	1.26096038	-0.48008075	2.61720114	C	-0.75766010	4.53836195	2.35104417
C	2.35288496	-0.48204841	1.81093403	C	1.12210940	3.03113524	2.07125820
C	3.36810411	-0.03713670	-0.21498488	H	-1.64734918	5.01345265	1.96024121
N	1.25835552	-1.29143139	5.06046412	C	-0.30894123	4.86575629	3.62167110
C	1.30914114	-0.92989390	3.96609047	H	-0.84695937	5.58537554	4.22047952
N	4.62451815	-1.34889424	2.68875973	C	0.85666264	4.28432395	4.10972266
C	3.60029187	-0.96217092	2.33058219	C	1.58350313	3.38244199	3.32661017
C	-3.16009996	0.03331192	-0.41350842	H	2.51910981	2.98888450	3.69706487
C	-2.37855860	-0.46622081	1.69896990	H	1.71116641	2.38178392	1.44098358
C	-0.50574386	-1.26854600	-2.62008590	H	-1.20675365	4.10567816	-0.16490045
C	-0.64927478	1.19987067	-2.60935563	H	-1.59410971	-1.21429051	-2.61421074
C	-0.83664061	2.26676334	-1.79143042	H	-0.20062488	-1.44114924	-3.65130653
C	-0.58383325	3.31468877	0.25083564	H	1.01054268	0.09572714	-2.35911903
N	-1.42277296	1.09721354	-5.06271222	H	4.24490436	-0.52929020	0.20398062
C	-1.08617986	1.19185224	-3.96330824	H	-1.42894393	-0.47787438	3.63031495
N	-2.04968818	4.37954112	-2.65570484	H	-0.96838218	-1.80281173	2.58091202
C	-1.50640766	3.42674559	-2.30368940	H	-0.09447572	0.98245252	2.37115837
C	0.53978864	-3.11836483	0.37970704	H	-5.76051520	-0.48209980	1.67344938
C	-0.05673361	-2.40095462	-1.73035501	C	-3.67547728	-0.58154091	2.18364127
H	-2.93075970	0.29448882	-1.43526624	H	-3.84242668	-0.81776574	3.22508708
C	-4.47897329	-0.07926047	-0.00943075	C	3.57111790	0.53113850	-1.52833828
H	-5.27505179	0.08305976	-0.72074475	C	4.62651762	0.01606864	-2.30111944
C	-4.74375856	-0.39282433	1.31797535				

Figure S99: Geometry optimized molecular Structure of **$[Ni(HL^{1\text{-}CF3})_2]^{2+}$.**

Table S1. Crystallographic parameters for **$Ni^{2\text{-}CF3}$, $Ni^{2\text{-}OMe}$, $Ni^{2\text{-}Mes}$** and **Co2-Mes.**

Compound	**$Ni^{2\text{-}CF3}$**	**$Ni^{2\text{-}OMe}$**	**$Ni^{2\text{-}Mes}$**	**$Co^{2\text{-}Mes}$**
Identification code	2838RKM_0m_a	Ni-2OMe	Ni-2Mes	Co-2Mes
Empirical formula	$C_{72}H_{44}F_{12}N_{20}Ni_2$	$C_{72}H_{53}N_{20}Ni_2O_4$	$C_{40}H_{36}N_{10}Ni$	$C_{40}H_{36}CoN_{10}$
Formula weight	1534.69	1379.76	715.48	715.72
Temperature/K	273.15	273.15	100	292.13
Crystal system	monoclinic	triclinic	monoclinic	monoclinic
Space group	$P2_1/c$	P-1	$P2_1/n$	$P2_1/n$
a/Å	14.5907(15)	11.5627(1)	14.8532(4)	14.9441(11)
b/Å	31.704(3)	18.1391(3)	12.1461(3)	12.2141(9)
c/Å	15.9226(16)	18.6743(3)	19.8214(5)	19.9191(15)
α/°	90	63.484(2)	90	90
β/°	107.430(2)	81.369(2)	100.771(3)	100.647(2)
γ/°	90	80.292(2)	90	90
Volume/$Å^3$	7027.3(12)	3442.07(10)	3512.95(16)	3573.2(5)
Z	4	2	4	4
$\rho_{calc}g/cm^3$	1.451	1.331	1.353	1.330
μ/mm^{-1}	0.626	0.611	0.598	0.525
F(000)	3120.0	1426.0	1496.0	1492.0
Crystal size/mm^3	0.2 × 0.12 × 0.11	0.2 × 0.15 × 0.1	0.11 × 0.1 × 0.09	0.28 × 0.15 × 0.11
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.202 to 50.182	4.142 to 51.728	3.16 to 50.2	4.338 to 50.07
Index ranges	-17 ≤ h ≤ 17, -37 ≤ k ≤ 37, -18 ≤ l ≤ 18	-13 ≤ h ≤ 13, -18 ≤ k ≤ 21, -22 ≤ l ≤ 22	-17 ≤ h ≤ 17, -14 ≤ k ≤ 12, -23 ≤ l ≤ 23	-17 ≤ h ≤ 17, -14 ≤ k ≤ 14, -23 ≤ l ≤ 23
Reflections collected	97002	39393	39707	47125
Independent reflections	12455 [R_{int} = 0.1408, R_{sigma} = 0.1008]	12084 [R_{int} = 0.0767, R_{sigma} = 0.0823]	6188 [R_{int} = 0.0578, R_{sigma} = 0.0342]	6288 [R_{int} = 0.0906, R_{sigma} = 0.0533]
Data/restraints/parameters	12455/0/925	12084/2/896	6188/0/467	6288/0/467
Goodness-of-fit on F^2	1.009	0.949	1.045	1.049
Final R indexes [I>=2σ (I)]	R_1 = 0.0737, wR_2 = 0.1651	R_1 = 0.0486, wR_2 = 0.1081	R_1 = 0.0429, wR_2 = 0.1129	R_1 = 0.0429, wR_2 = 0.1064
Final R indexes [all data]	R_1 = 0.1358, wR_2 = 0.1953	R_1 = 0.0847, wR_2 = 0.1263	R_1 = 0.0558, wR_2 = 0.1207	R_1 = 0.0624, wR_2 = 0.1194
Largest diff. peak/hole / e $Å^{-3}$	0.91/-0.81	0.35/-0.33	1.05/-0.91	0.66/-0.49

Table S2. Crystallographic parameters for $\mathbf{Co^{1\text{-}CF3}}$, $\mathbf{Co^{1\text{-}OMe}}$, $\mathbf{Co^{2\text{-}CF3}.BPh_4}$ and $\mathbf{Co^{2\text{-}OMe}.ClO_4}$.

Compound	$\mathbf{Co^{1\text{-}CF3}}$	$\mathbf{Co^{1\text{-}OMe}}$	$\mathbf{Co^{2\text{-}CF3}.BPh_4}$	$\mathbf{Co^{2\text{-}OMe}.ClO_4}$
Identification code	Co-1CF3	Co-1OMe	Co-2CF3_BPh4	Co-2OMe_ClO4
Empirical formula	$C_{36}H_{22}CoF_6N_{10}$	$C_{36}H_{28}CoN_{10}O_2$	$C_{60}H_{42}BCoF_6N_{10}$	$C_{39}H_{32.5}ClCoN_{11.5}O_6$
Formula weight	767.567	691.61	1086.77	852.64
Temperature/K	273.15	298	273.15	100.0
Crystal system	monoclinic	monoclinic	triclinic	triclinic
Space group	$P2_1/n$	$P2_1/c$	P-1	P-1
a/Å	18.6410(9)	17.736(7)	10.8487(9)	10.0065(2)
b/Å	7.9755(4)	8.011(3)	13.9831(12)	13.3202(3)
c/Å	24.6464(11)	23.631(9)	18.4002(15)	15.2558(4)
α/°	90	90	91.7250(10)	97.7210(10)
β/°	107.811(1)	97.083(8)	90.4220(10)	105.4330(10)
γ/°	90	90	110.7980(10)	95.6980(10)
Volume/$Å^3$	3488.6(3)	3332(2)	2607.7(4)	1922.83(8)
Z	4	4	2	2
$\rho_{calc}g/cm^3$	1.461	1.379	1.384	1.473
μ/mm^{-1}	0.567	0.565	0.402	4.679
F(000)	1558.3	1428.0	1116.0	878.0
Crystal size/mm^3	0.25 × 0.21 × 0.18	0.13 × 0.12 × 0.1	0.26 × 0.18 × 0.08	0.22 × 0.18 × 0.14
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	CuKα (λ = 1.54178)
2Θ range for data collection/°	3.48 to 50.16	3.474 to 55.718	3.76 to 54.524	6.096 to 150.176
Index ranges	$-22 \le h \le 22$, $-9 \le k \le 9$, $-29 \le l \le 29$	$-21 \le h \le 21$, $-10 \le k \le 10$, $-29 \le l \le 28$	$-13 \le h \le 13$, $-17 \le k \le 17$, $-23 \le l \le 23$	$-12 \le h \le 12$, $-16 \le k \le 16$, $-19 \le l \le 18$
Reflections collected	94897	58316	72840	68746
Independent reflections	6167 [R_{int} = 0.1021, R_{sigma} = 0.0374]	6885 [R_{int} = 0.1257, R_{sigma} = 0.0943]	11647 [R_{int} = 0.1030, R_{sigma} = 0.0779]	7573 [R_{int} = 0.0703, R_{sigma} = 0.0371]
Data/restraints/parameters	6167/96/532	6885/0/445	11647/0/704	7573/0/545
Goodness-of-fit on F^2	1.103	0.991	0.944	1.058
Final R indexes [I>=2σ (I)]	R_1 = 0.0480, wR_2 = 0.1052	R_1 = 0.0465, wR_2 = 0.1071	R_1 = 0.0503, wR_2 = 0.1242	R_1 = 0.0473, wR_2 = 0.1228
Final R indexes [all data]	R_1 = 0.0674, wR_2 = 0.1173	R_1 = 0.1218, wR_2 = 0.1372	R_1 = 0.0826, wR_2 = 0.1376	R_1 = 0.0510, wR_2 = 0.1259
Largest diff. peak/hole / e $Å^{-3}$	0.41/-0.36	0.34/-0.53	0.77/-0.56	0.57/-0.79

Table S3. Crystallographic parameters for **$Zn^{1\text{-}Mes}$**.

Compound	**$Zn^{1\text{-}Mes}$**
Identification code	Zn-1-Mes
Empirical formula	$C_{40}H_{36}N_{10}Zn$
Formula weight	722.16
Temperature/K	273.15
Crystal system	monoclinic
Space group	C2/c
a/Å	18.469(4)
b/Å	8.4743(14)
c/Å	23.805(4)
α/°	90
β/°	98.031(4)
γ/°	90
Volume/$Å^3$	3689.2(11)
Z	4
$\rho_{calc}g/cm^3$	1.300
μ/mm^{-1}	0.709
F(000)	1504.0
Crystal size/mm^3	0.2 × 0.1 × 0.08
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	6.008 to 50.01
Index ranges	$-21 \leq h \leq 21$, $-10 \leq k \leq 10$, $-28 \leq l \leq 28$
Reflections collected	18514
Independent reflections	3231 [R_{int} = 0.0522, R_{sigma} = 0.0296]
Data/restraints/parameters	3231/0/234
Goodness-of-fit on F^2	1.125
Final R indexes [I>=2σ (I)]	R_1 = 0.0439, wR_2 = 0.1043
Final R indexes [all data]	R_1 = 0.0499, wR_2 = 0.1072
Largest diff. peak/hole / e $Å^{-3}$	0.34/-0.30

Table S4. Selected bond distance (Å) obtained from DFT calculated structures.

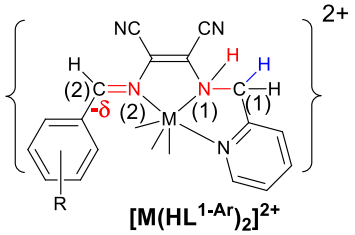
	Complex	M – N(1)	M– N(2)	C(1)– N(1)	C(2)–N(2)
 $[M(HL^{1\text{-}Ar})_2]^{2+}$	$HL^{1\text{-}Mes}$	------	------	1.445	1.291
	$HL^{1\text{-}OMe}$	------	------	1.444	1.287
	$HL^{1\text{-}CF3}$	------	------	1.446	1.284
	$[Co(HL^{1\text{-}Mes})_2]^{2+}$	2.164	2.312	1.485	1.320
	$[Co(HL^{1\text{-}OMe})_2]^{2+}$	2.157	2.308	1.491	1.318
	$[Co(HL^{1\text{-}CF3})_2]^{2+}$	2.170	2.388	1.487	1.304
	$[Ni(HL^{1\text{-}Mes})_2]^{2+}$	2.094	2.298	1.489	1.308
	$[Ni(HL^{1\text{-}OMe})_2]^{2+}$	2.108	2.284	1.508	1.319
	$[Ni(HL^{1\text{-}CF3})_2]^{2+}$	2.109	2.326	1.490	1.303

Figure S100: Kinetic data for the reaction of **$Ni(ClO_4)_2.6H_2O$** (1.8×10^{-5}M) and **$HL^{1\text{-}Mes}$** (3.6×10^{-5}M) in acetonitrile to the formation of **$Ni^{2\text{-}Mes}$**

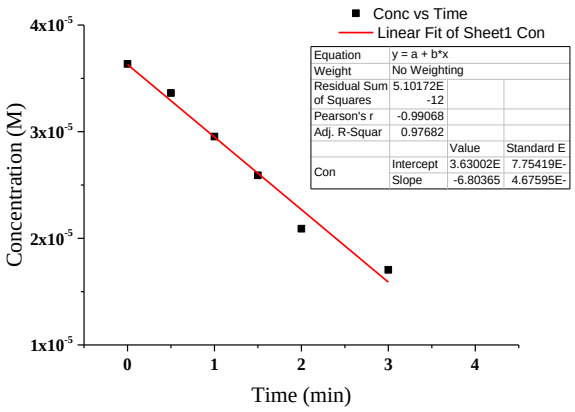
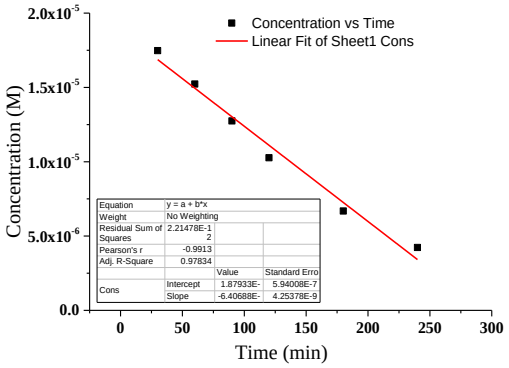
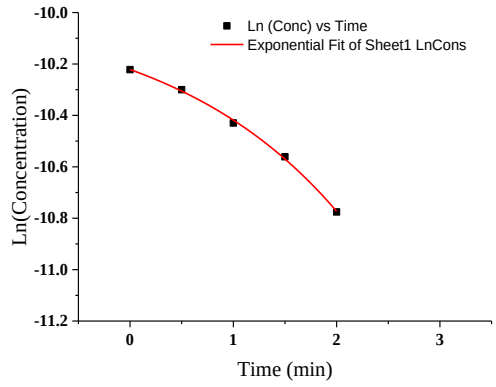
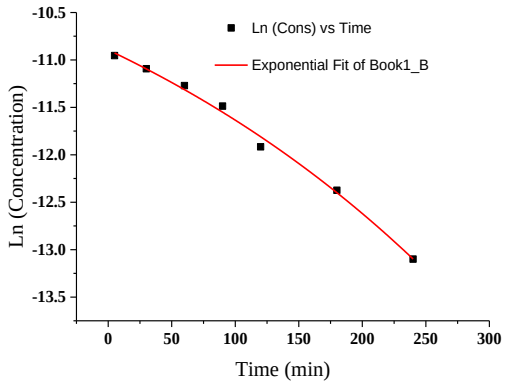
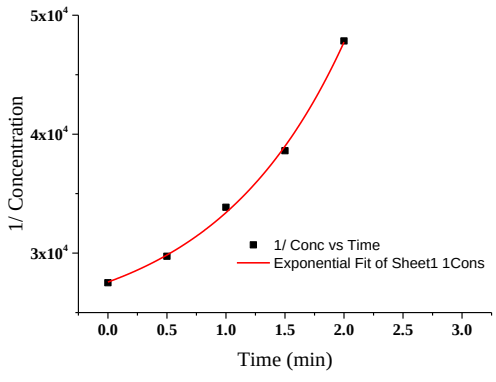
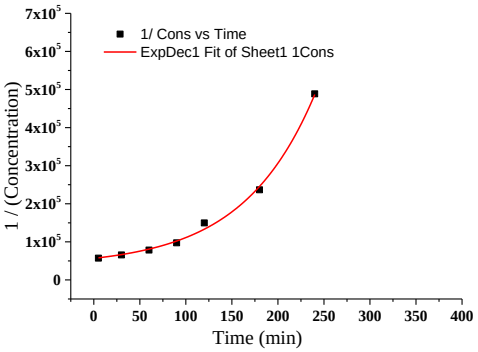
Step-I	**Step-II**
Plot of concentration vs. time	**Plot of concentration vs. time**
	
Plot of Ln(concentration) vs. time	**Plot of Ln(concentration) vs. time**
	
Plot of 1/concentration vs. time	**Plot of 1/concentration vs. time**
	

Figure S101: Kinetic data for the reaction of **$Co(ClO_4)_2.6H_2O$** (1.2×10^{-5}M) and **$HL^{1\text{-}Mes}$** (2.4×10^{-5}M) in acetonitrile to the formation of **$Co^{2\text{-}Mes}$**

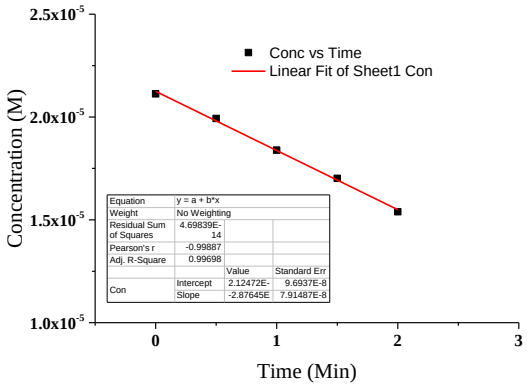
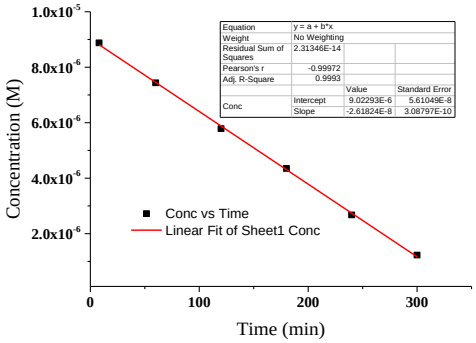
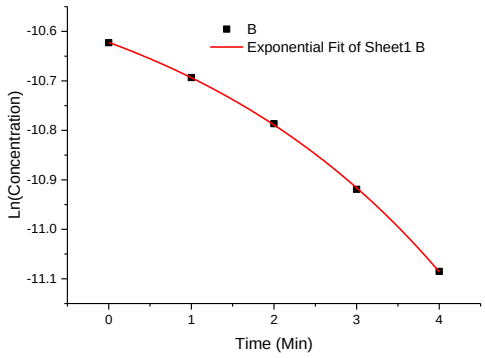
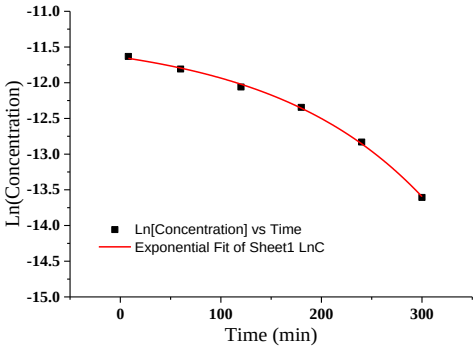
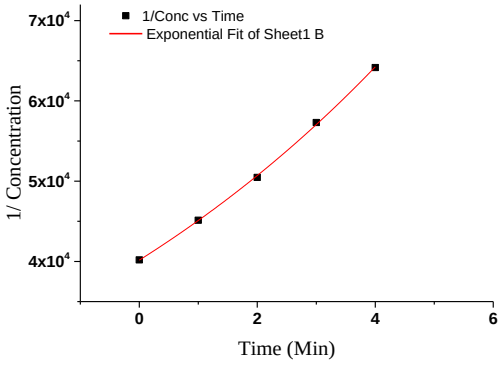
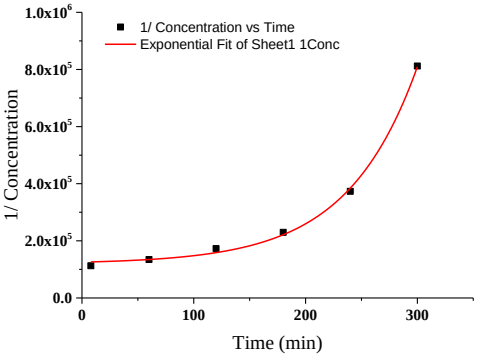
Step-I	**Step-II**
Plot of concentration vs. time	**Plot of concentration vs. time**
	
Plot of Ln(concentration) vs. time	**Plot of Ln(concentration) vs. time**
	
Plot of 1/concentration vs. time	**Plot of 1/concentration vs. time**
	

Figure S102: Kinetic data for the reaction of **$Ni(ClO_4)_2.6H_2O$** (1.05×10^{-5}M) and **$HL^{1\text{-}CF3}$** (2.1×10^{-5}M) in acetonitrile to the formation of **$Ni^{2\text{-}CF3}$**

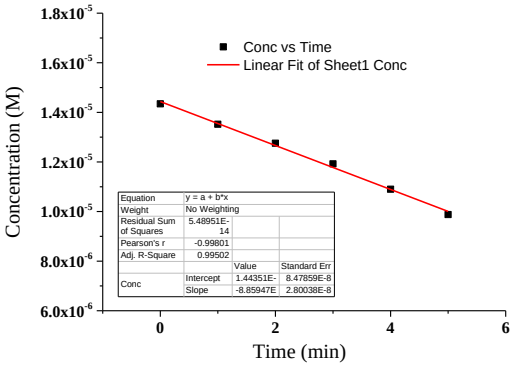
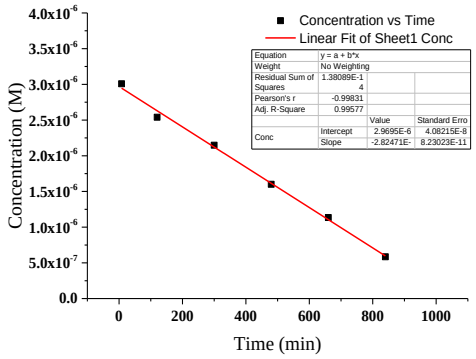
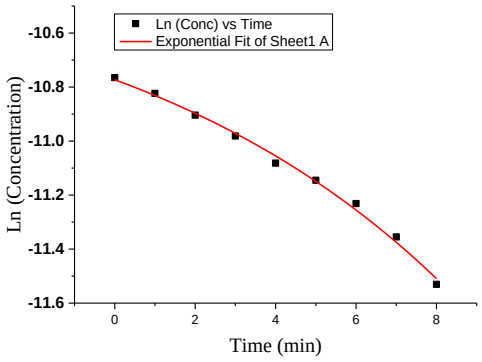
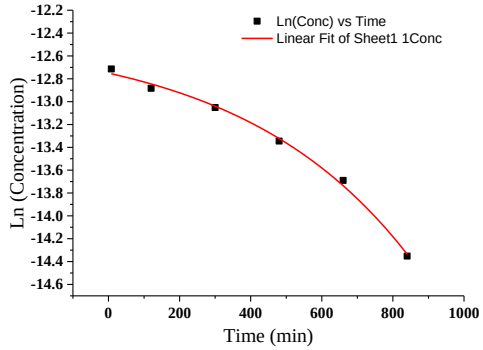
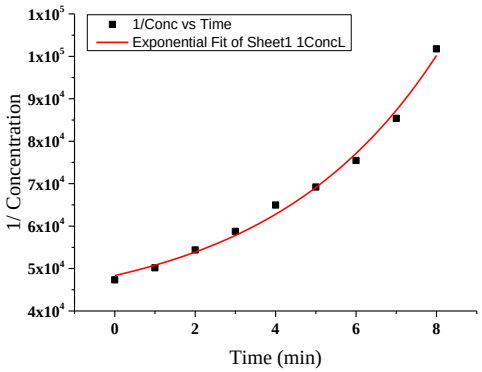
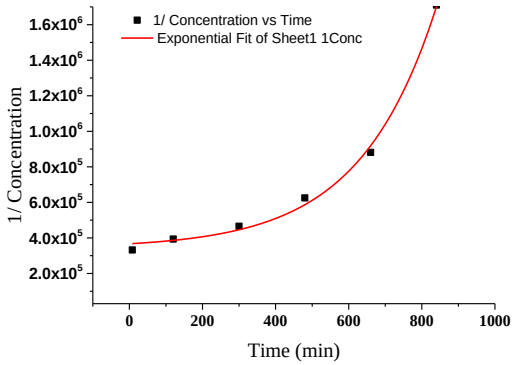
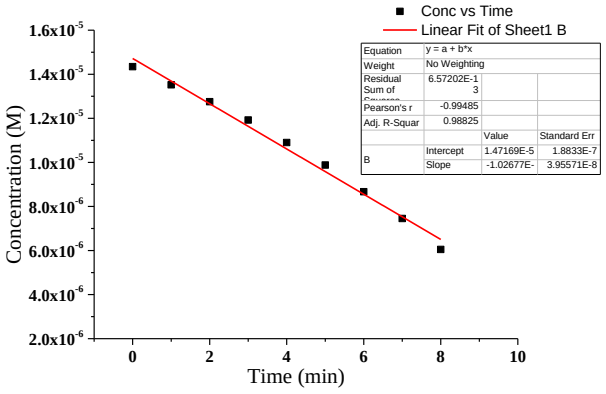
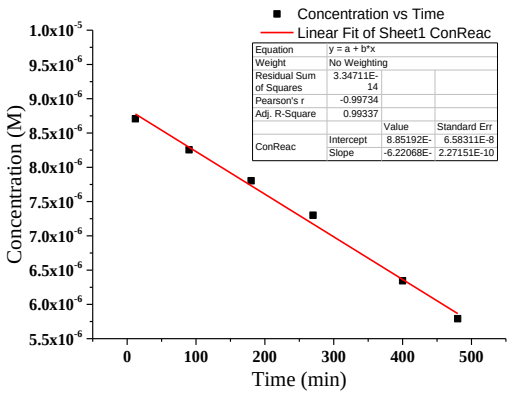
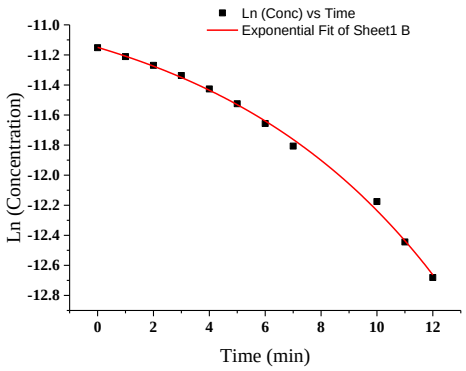
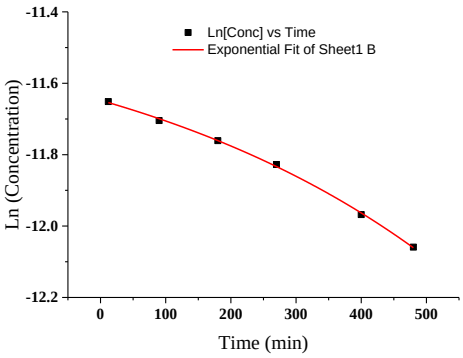
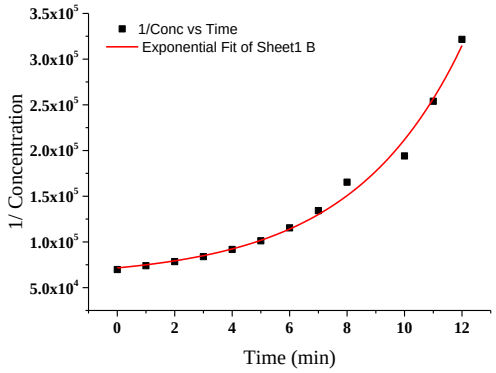
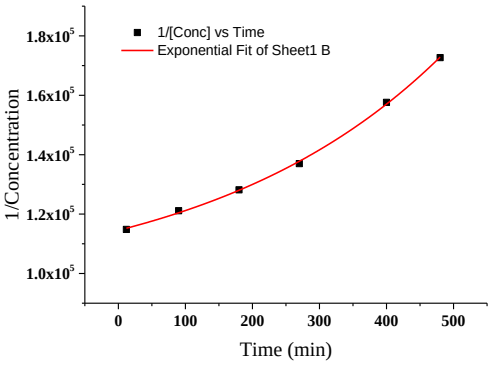
Step-I	**Step-II**
Plot of concentration vs. time	**Plot of concentration vs. time**
	
Plot of Ln(concentration) vs. time	**Plot of Ln(concentration) vs. time**
	
Plot of 1/concentration vs. time	**Plot of 1/concentration vs. time**
	

Figure S103: Kinetic data for the reaction of **$Ni(ClO_4)_2.6H_2O$** (7.16 x10^{-6}M) and **$HL^{1\text{-}OMe}$** (1.43 x 10^{-5} M) in acetonitrile to the formation of **$Ni^{2\text{-}OMe}$**

Step-I	**Step-II**
Plot of concentration vs. time	**Plot of concentration vs. time**
	
Plot of Ln(concentration) vs. time	**Plot of Ln(concentration) vs. time**
	
Plot of 1/concentration vs. time	**Plot of 1/concentration vs. time**
	

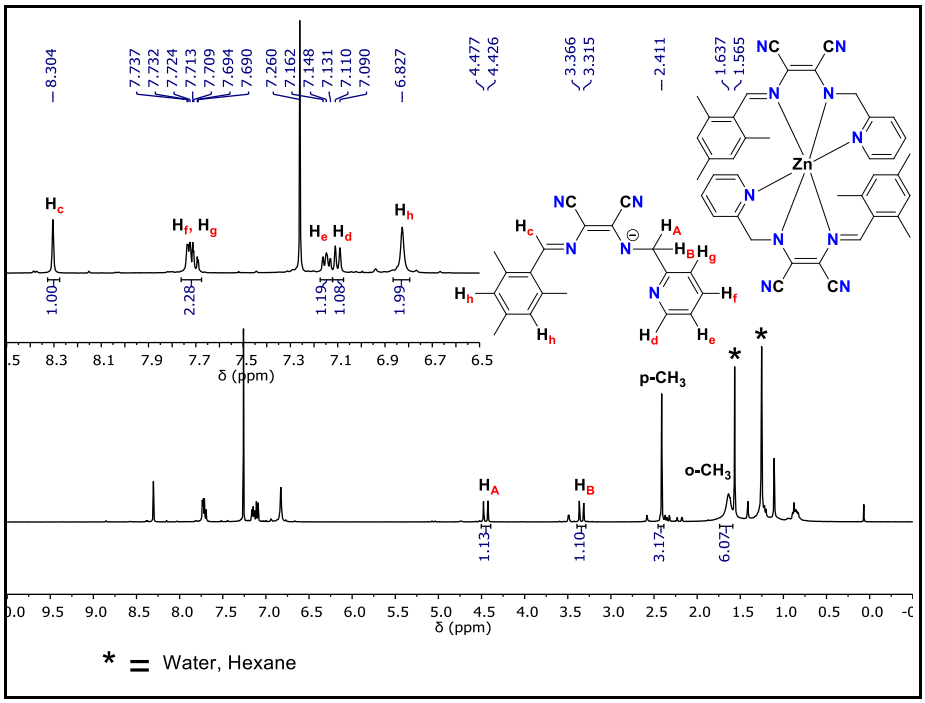


Figure S104: ^{1}H NMR Spectrum of **Zn$^{1\text{-Mes}}$** in $CDCl_3$.

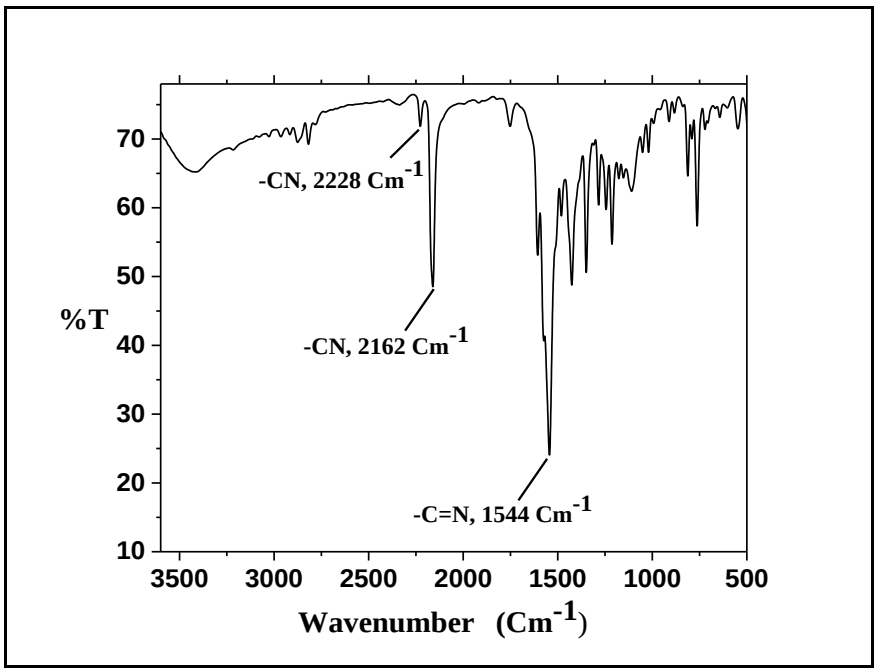


Figure S105: FTIR Spectrum of **Zn$^{1\text{-Mes}}$** .

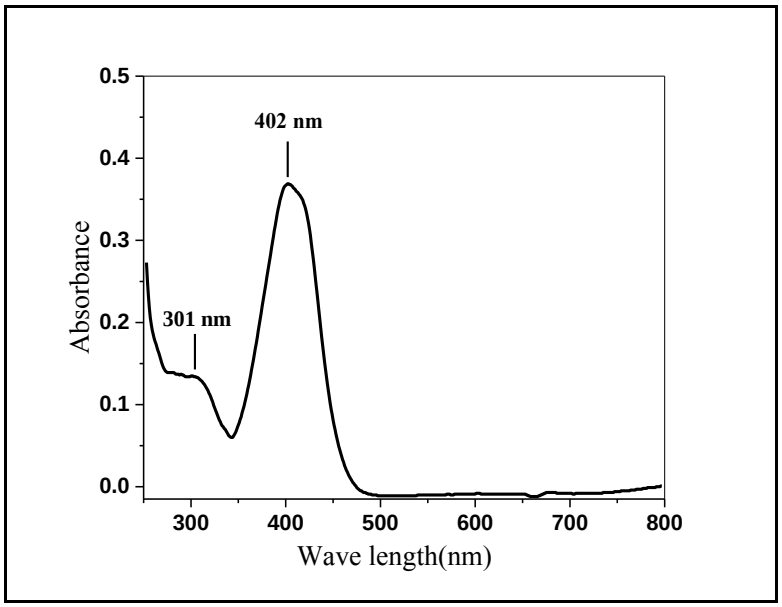


Figure S105: Electronic absorption Spectrum of $\mathbf{Zn^{1\text{-}Mes}}$ (10^{-5} M) in acetonitrile.