Selective colorimetric sensing of Co(II) in aqueous media with a spiropyran-amide-dipicolylamine linkage under UV irradiation

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Electronic Supplementary Information (ESI†)

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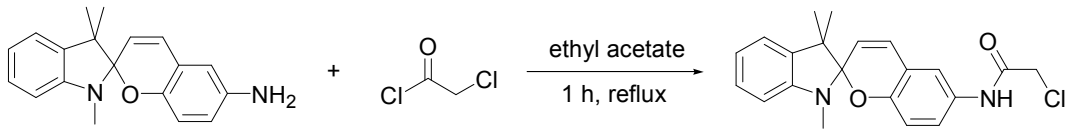
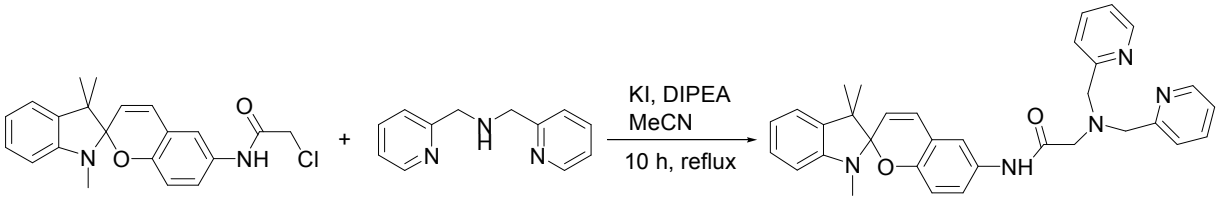
Experimental

Synthesis



3 2

Synthesis of 2: 3[1] (1.59 g, 5.4 mmol) and 2-chloroacetyl chloride (790 mg, 7.0 mmol) were refluxed in ethyl acetate (15 ml) for 1 h under nitrogen atmosphere and concentrated by evaporation. The residue was purified by recrystallization with $CHCl_3$, affording **2** as a red solid (1.91 g, 75 %). ^{1}H NMR (270 MHz, DMSO-d_6, TMS): δ = 1.76 (s, 6H, –C(CH_3)$_2$), 4.08 (s, 3H, N-CH_3), 4.29 (s, 2H, C=O-CH_2-Cl), 7.12 (d, J = 8.74 Hz, 1H, Ar–*H*), 7.53–7.66 (m, 4H, Ar–*H*), 7.84–7.92 (m, 2H, Ar–*H*), 8.20 (s, 1H, –C*H*CNH), 8.45 (d, J = 16.3 Hz, 1H, N(CH$_3$)-C-CH-C*H*), 10.47 (s, 1H, N*H*). ^{13}C NMR (100 MHZ, DMSO-d_6, TMS): δ = 25.8, 34.1, 43.2, 51.8, 112.3, 115.0, 117.1, 120.7, 121.1, 122.7, 128.1, 128.9, 129.1, 130.6, 141.8, 143.1, 148.2, 156.0, 164.5, 181.7. FAB-MS: m/z: calcd for $C_{21}H_{21}ClN_2O_2$: 368.1; found: 369.2 [M + H$^+$]; HR-MS (FAB): m/z: calcd for $C_{21}H_{22}ClN_2O_2$ [M + H$^+$]: 369.1370; found: 369.1389.



2 1

Synthesis of 1: 2 (110 mg, 0.30 mmol), di-2-picolylamine (70 mg, 0.35 mmol), KI (30 mg), and diisopropylethylamine (DIPEA) (0.5 ml) were added to MeCN (40 ml), and the solution was refluxed for 10 h under nitrogen atmosphere. The resultant was concentrated by evaporation and purified by silica gel column chromatography (ethyl acetate/MeOH, 10/1), affording **1** as a red solid (103 mg, 65 %). ^{1}H NMR (270 MHz, CD_3CN-d_3, TMS): δ = 1.13 (s, 3H, –C(CH_3)$_2$), 1.26 (s, 3H, –C(CH_3)$_2$), 2.69 (s, 3H, N-CH_3), 3.38 (s, 2H, C=O-CH_2-N), 3.89 (s, 4H, N-CH_2-py), 5.78 (d, J = 10.2 Hz, 1H, –CC*H*CH), 6.52–6.59 (m, 2H, Ar–*H*), 6.80 (t, J = 7.4 Hz, 1H, Ar–*H*), 6.95 (d, J = 10.2 Hz, 1H, –CCHC*H*–), 7.07–7.16 (m, 2H, Ar–*H*), 7.19–7.24 (m, 2H, Ar–*H*), 7.33 (d, J = 7.8 Hz, 2H, Ar–*H*), 7.37 (dd, J = 2.6, 8.7 Hz, 1H, Ar–*H*), 7.55 (d, J = 2.5 Hz, 1H, Ar–*H*), 7.64–7.70 (m, 2H, Ar–*H*), 8.56–8.58 (m, 2H, Ar–*H*), 10.60 (s, 1H, N*H*). ^{13}C NMR (68 MHZ, DMSO-d_6, TMS): δ = 19.9, 25.6, 28.5, 51.2, 57.6, 59.3, 103.5, 106.5, 114.2, 117.7, 118.2, 118.7, 119.7, 120.8, 121.2, 122.3, 122.9, 127.2, 129.1, 131.3, 136.0, 136.6, 147.6, 148.7, 149.8, 157.9, 168.3. FAB-MS: m/z: calcd for $C_{33}H_{33}N_5O_2$: 531.3; found: 532.2 [M + H$^+$]; HR-MS (FAB): m/z: calcd for $C_{33}H_{34}N_5O_2$ [M + H$^+$]: 532.2713; found: 532.2720.

Methods

Absorption spectra were measured in an aerated condition using a 10 mm path length quartz cell on an UV-visible photodiode-array spectrophotometer (Shimadzu; Multispec-1500) equipped with a temperature controller S-1700. Light irradiations (280 nm and 450 nm) were carried out with a Xenon lamp (300 W; Asahi Spectra Co. Ltd.; MAX-302) equipped with band-pass filters. The intensities of 280 nm and 450 nm light are 69.1 mW m^{-2} and 42.8 mW m^{-2}, respectively. ^{1}H and ^{13}C NMR spectra were obtained by a JEOL JNM-GSX270 Excalibur and JNM-AL400 spectrometer. FAB- and ESI-MS spectra were obtained by a JEOL JMS 700 Mass Spectrometer. Infrared spectra were recorded at room temperature using a FTIR–610 spectrometer (Jasco Corp.) with a liquid sample cell with a CaF_2 window.

Calculation details

Preliminary geometry optimizations were performed using the WinMOPAC version 3.0 software (Fujitsu Inc.) at the semiempirical PM3 level.[2] The obtained structures were fully refined with the convergence criteria at the DFT level with the Gaussian 03 package,[3] using the B3LYP/3-21G basis set. The excitation energies and the oscillator strength of each structure were calculated by the time-dependent density-functional response theory (TD-DFT)[4] at the same level of optimization using the polarizable continuum model (PCM)[5] with water as a solvent. Cartesian coordinates for compounds are summarized in the end of ESI†.

References

[1] T. Zimmermann, O. Brede, *J. Heterocyclic Chem*., **2003**, *40*, 611–616.

[2] Y. Shiraishi, N. Saito, T. Hirai *J. Am. Chem. Soc.*, **2005**, *127*, 8304–8306.

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[4] R. E. Stratmann, G. E. Scuseria, M. J. Frisch, *J. Chem. Phys.,* **1998**, *109*, 8218–8224.

[5] M. Cossi, V. Barone, R. Cammi, J. Tomasi, *Chem. Phys. Lett.,* **1996**, *255*, 327–335.

Table S1. Calculated excitation energy (*E*), wavelength (λ) and oscillator strength (*f*) for low-laying singlet state (S_n) of **1**(MC).

	Main orbital transition (CIC[a])	*E* (eV) [λ (nm)]	*F*
$S_0 \rightarrow S_1$	HOMO→LUMO (0.61)	2.6408 [469.49]	0.9302
$S_0 \rightarrow S_2$	HOMO-3→LUMO (0.66) HOMO-2→LUMO (-0.17) HOMO-1→LUMO (-0.10)	2.9142 [425.45]	0.0001
$S_0 \rightarrow S_3$	HOMO-3→LUMO (0.10) HOMO-1→LUMO (0.69)	3.2556 [380.83]	0.0535

[a]CI expansion coefficients for the main orbital transitions.

Table S2. Interfacial plots of key molecular orbitals of **1**(MC).

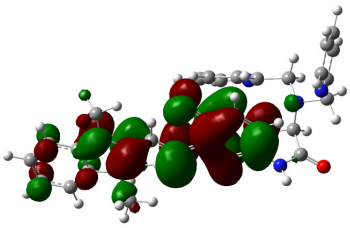
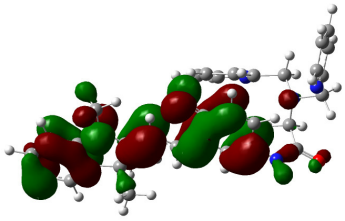
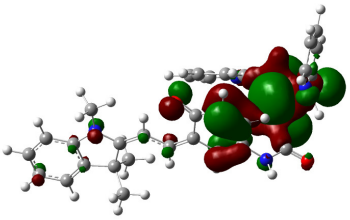
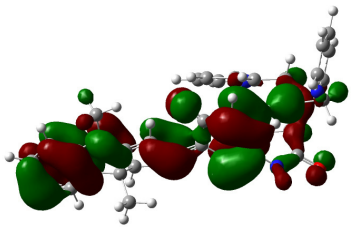
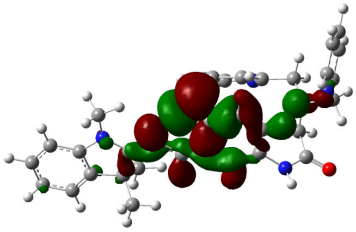
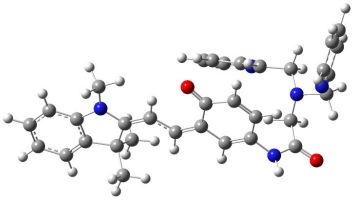
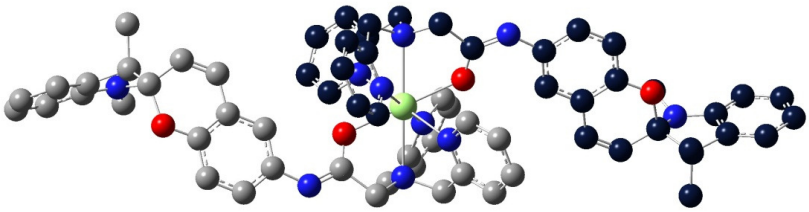
LUMO	HOMO	HOMO-1
		
HOMO-2	**HOMO-3**	
		

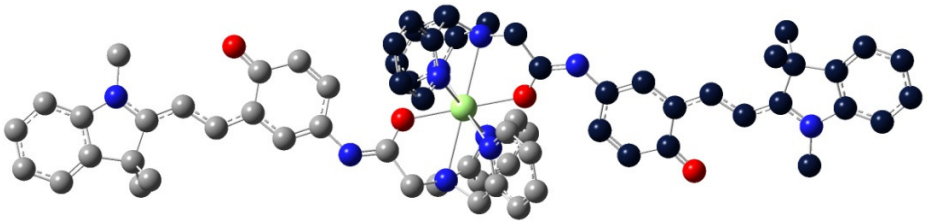
Table S3. Bond lengths for metal-ligand coordination.

2:1 **1**(SP)–Co^{2+} complex



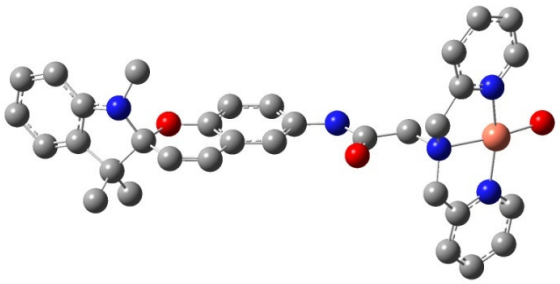
	Å		Å
Co^{2+}–N_{amine}	2.64427	Co^{2+}–N_{amine}'	2.60387
Co^{2+}–$N_{pyridine}$	2.35411	Co^{2+}–$N_{pyridine}'$	2.35357
Co^{2+}–$N_{pyridine}$	2.38778	Co^{2+}–$N_{pyridine}'$	2.39741
Co^{2+}–O	2.18546	Co^{2+}–O′	2.19487
amide C=O	1.28994		

2:1 **1**(MC)–Co^{2+} complex



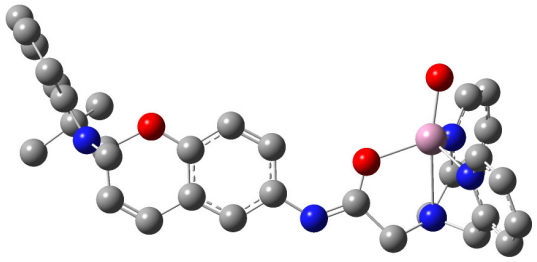
	Å		Å
Co^{2+}–N_{amine}	2.62733	Co^{2+}–N_{amine}'	2.60559
Co^{2+}–$N_{pyridine}$	2.35461	Co^{2+}–$N_{pyridine}'$	2.34568
Co^{2+}–$N_{pyridine}$	2.39589	Co^{2+}–$N_{pyridine}'$	2.39949
Co^{2+}–O	2.18927	Co^{2+}–O′	2.19571
amide C=O	1.27441		

1:1 **1**(SP)–Cu^{2+} complex



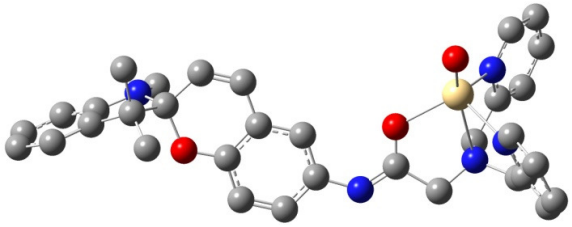
	Å		Å
Cu^{2+}–N_{amine}	2.09511	Cu^{2+}–$N_{pyridine}$	1.98067
Cu^{2+}–$N_{pyridine}$	1.98067	amide C=O	1.25274

1:1 **1**(SP)–Zn^{2+} complex



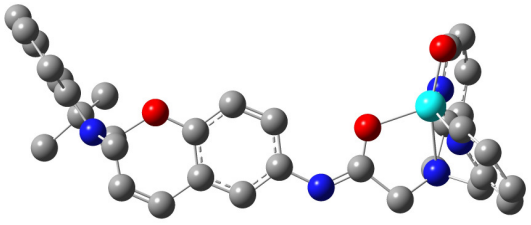
	Å		Å
Zn^{2+}–N_{amine}	2.45833	Zn^{2+}–$N_{pyridine}$	2.14870
Zn^{2+}–$N_{pyridine}$	2.10947	Zn^{2+}–O	2.05082
amide C=O	1.27091		

1:1 **1**(SP)–Cd^{2+} complex



	Å		Å
Cd^{2+}–N_{amine}	2.54979	Cd^{2+}–$N_{pyridine}$	2.33312
Cd^{2+}–$N_{pyridine}$	2.33155	Cd^{2+}–O	2.28189
amide C=O	1.27052		

1:1 **1**(SP)–Ni^{2+} complex



	Å		Å
Ni^{2+}–N_{amine}	2.19157	Ni^{2+}–$N_{pyridine}$	2.10477
Ni^{2+}–$N_{pyridine}$	2.07245	Ni^{2+}–O	2.03796
amide C=O	1.27012		

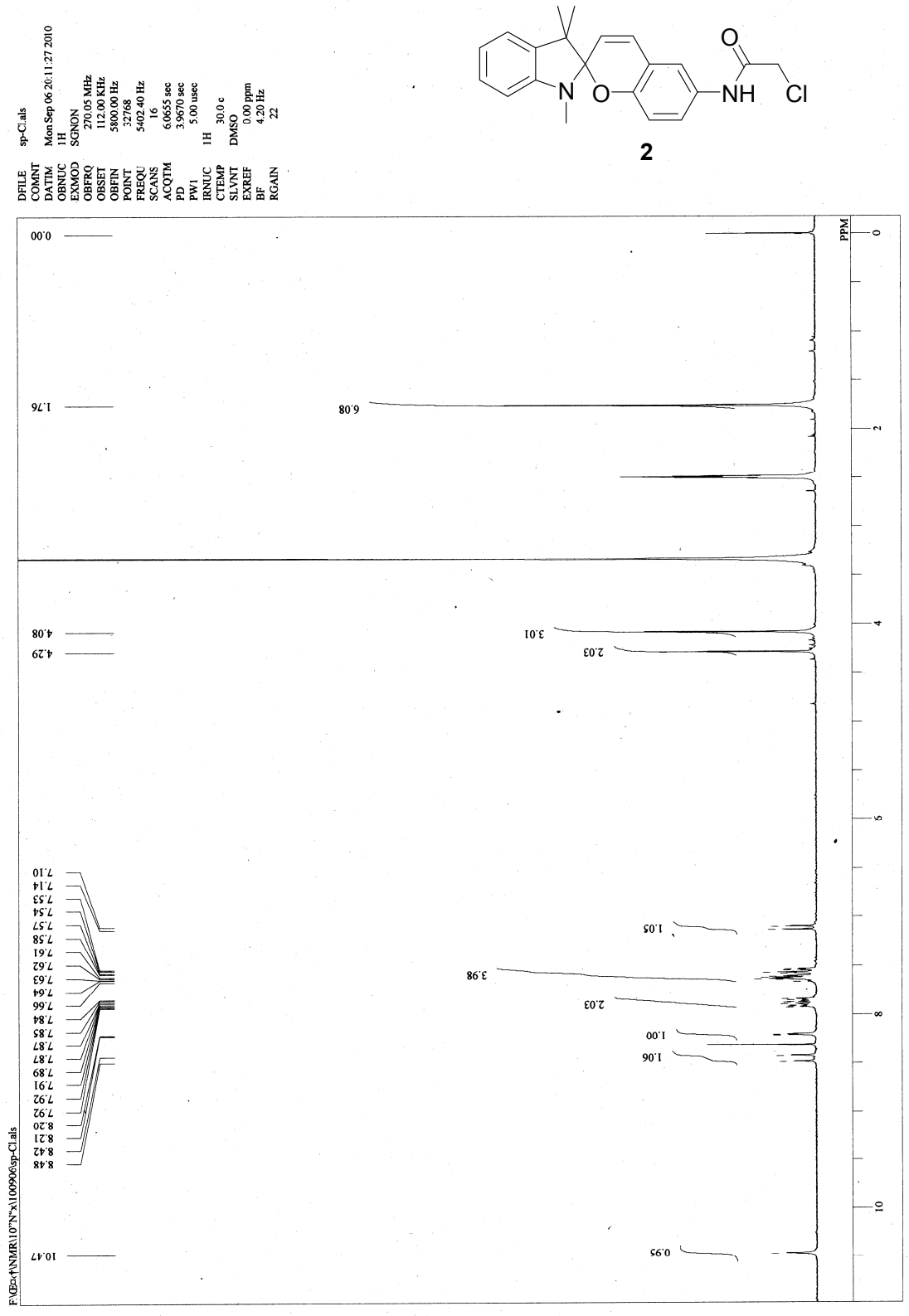


Fig. S1 ^{1}H NMR chart of **2** (DMSO-d_6, 270 MHz).

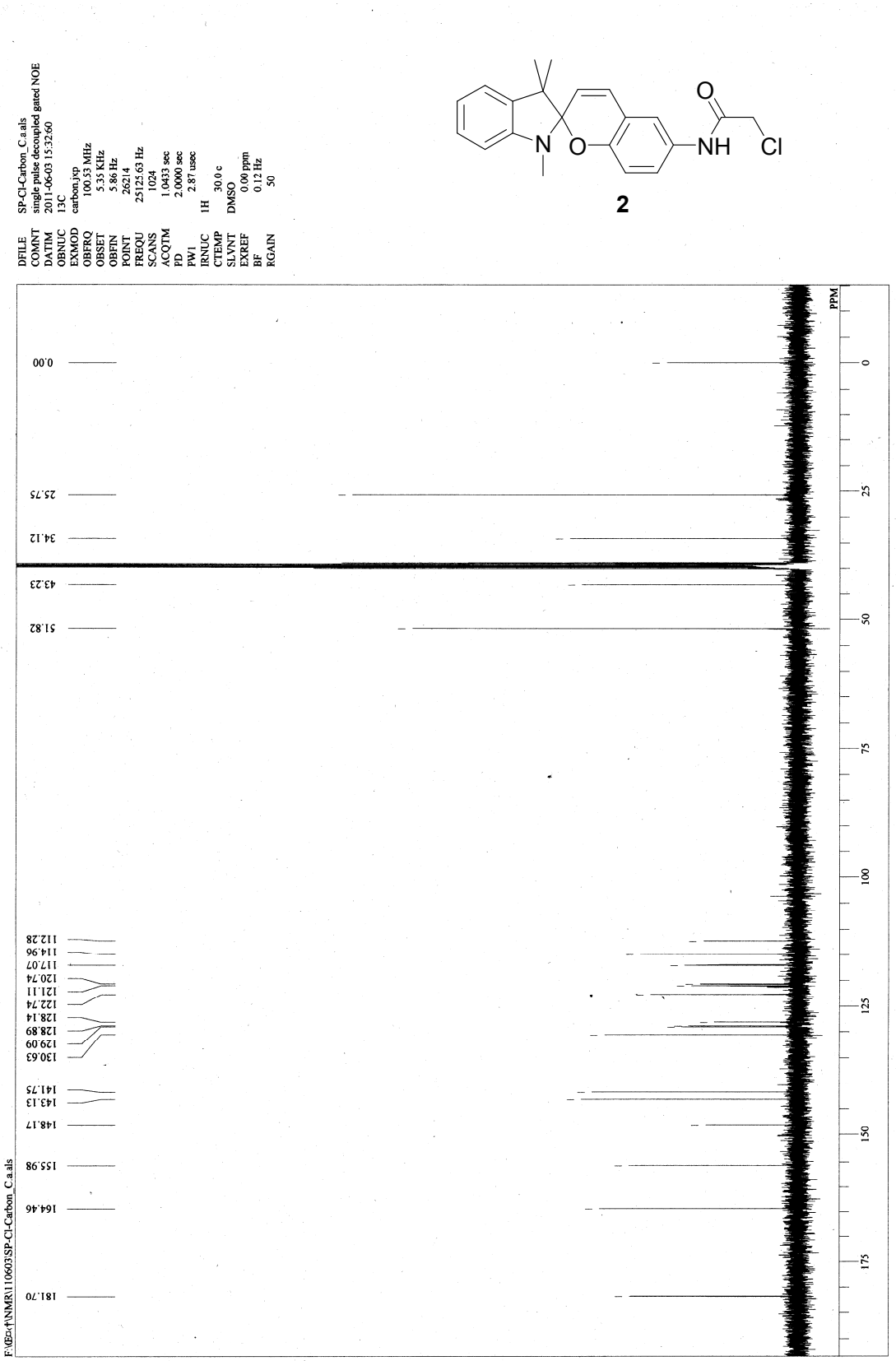


Fig. S2 ^{13}C NMR chart of **2** (DMSO-d_6, 100 MHz)**.**

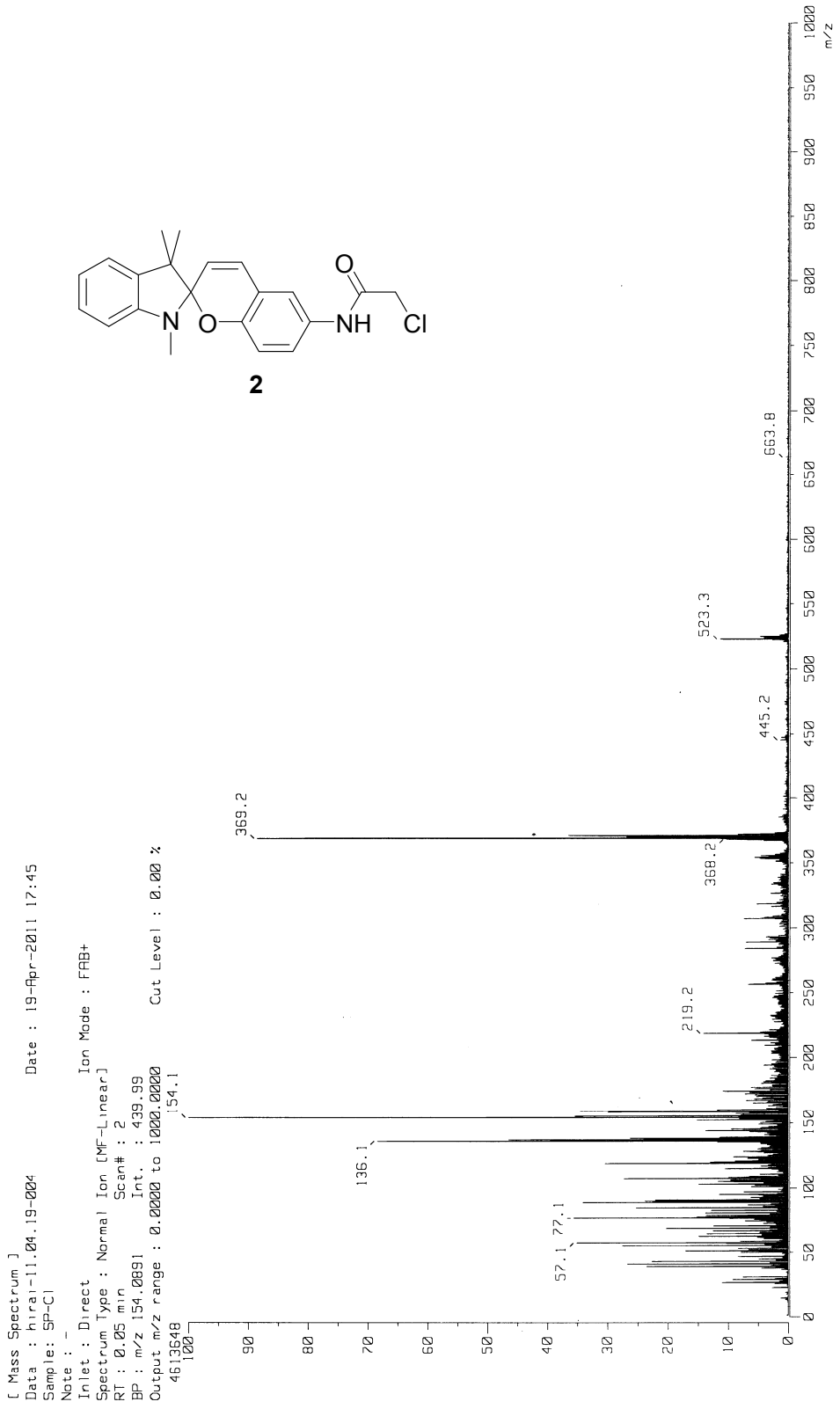


Fig. S3 FAB-MS chart of **2.**

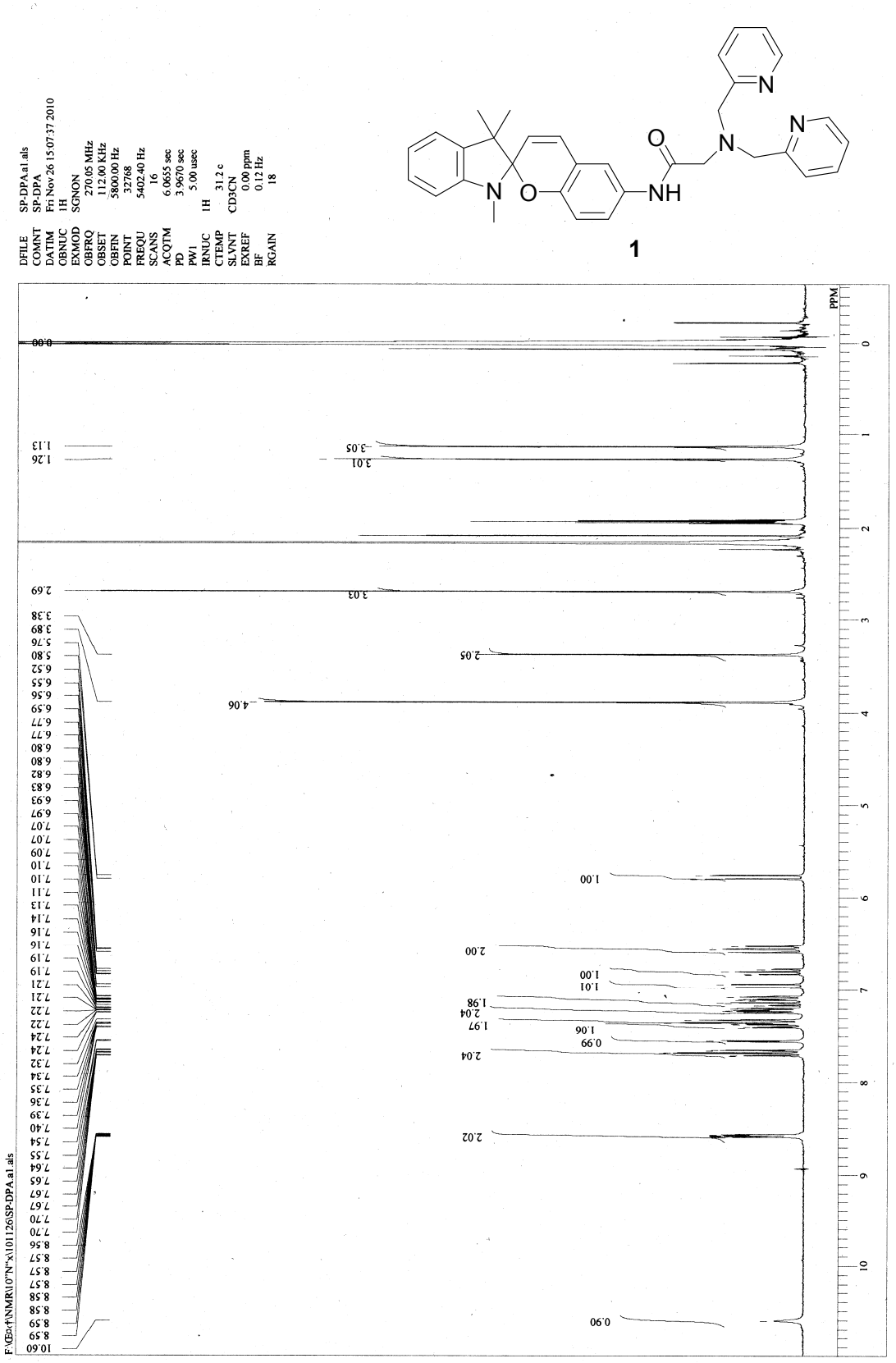
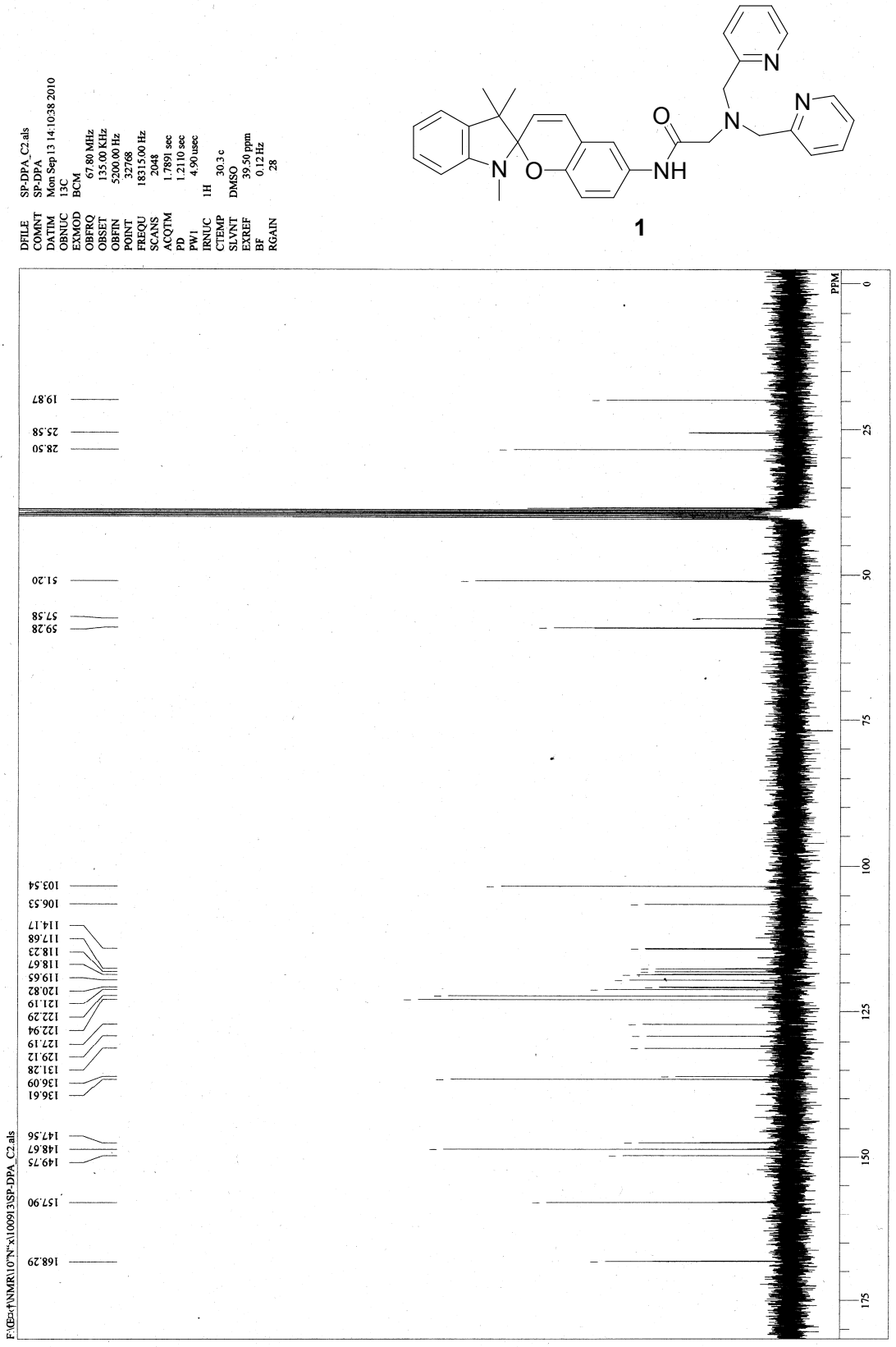


Fig. S4 ^{1}H NMR chart of **1** (CD_3CN-d_3, 270 MHz).



1

Fig. S5 ^{13}C NMR chart of **1** (DMSO-d_6, 68 MHz)**.**

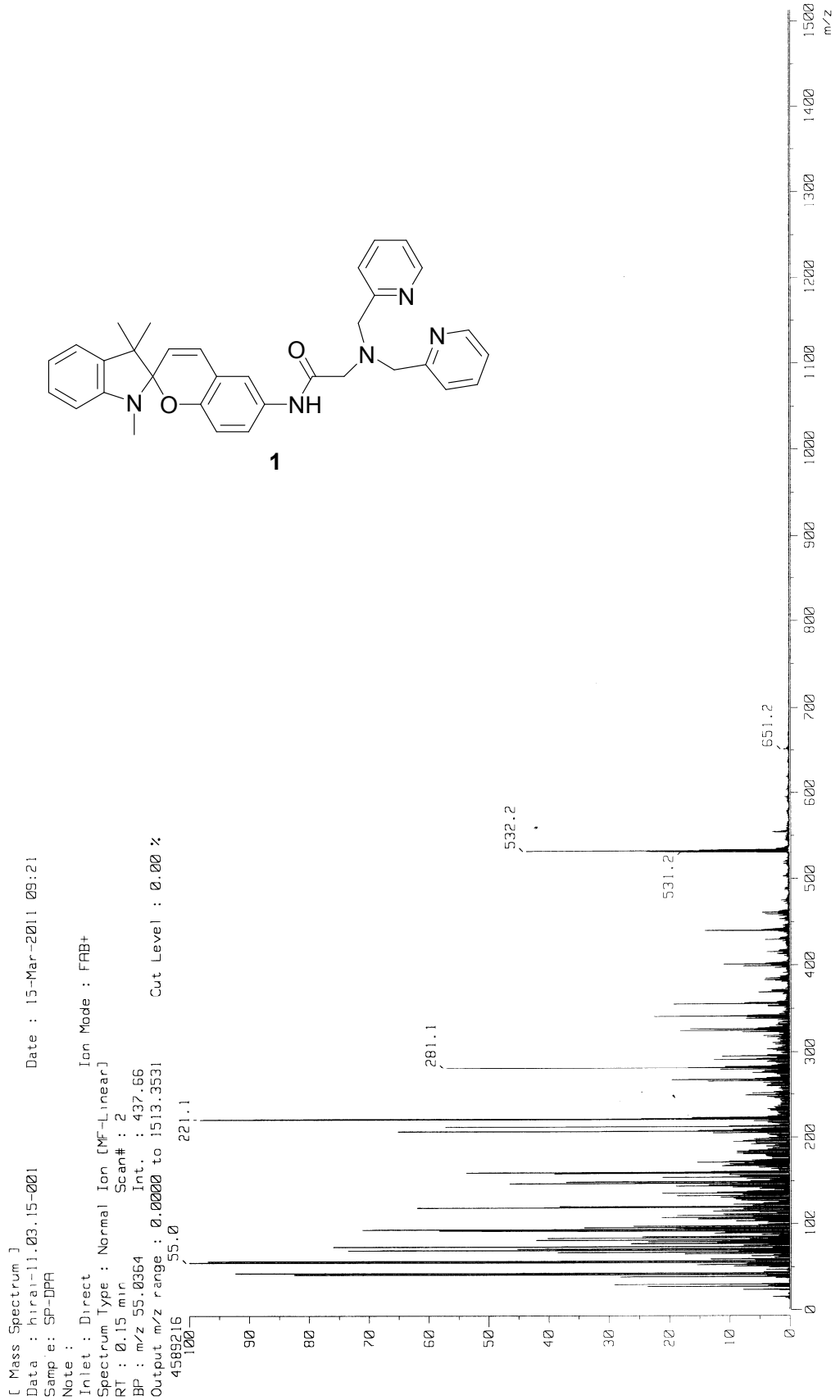


Fig. S6 FAB-MS chart of **1.**

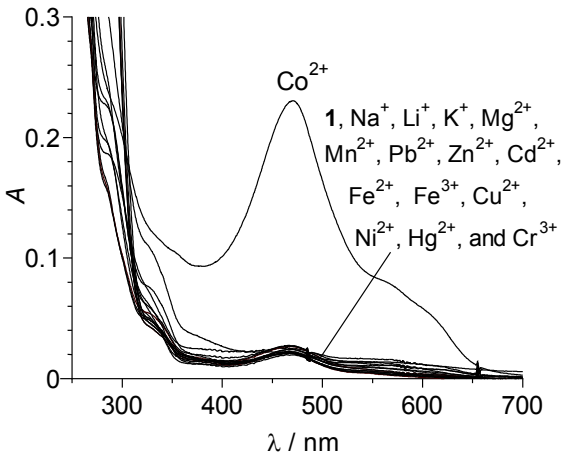


Fig. S7 Absorption spectra of **1** (20 μM) measured in a water/MeCN mixture (1/1 v/v; pH 7.4) with respective metal cations (1 equiv) after UV irradiation (280 nm) for 1 h.

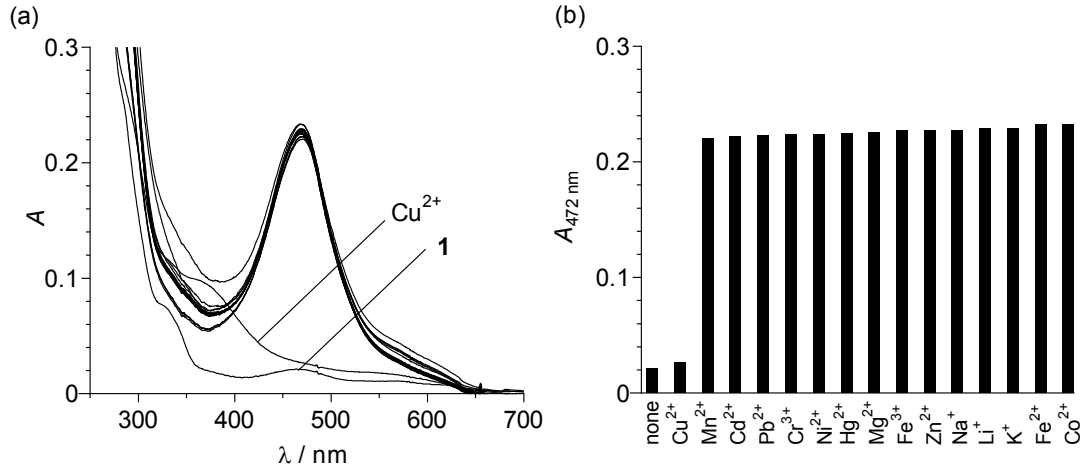


Fig. S8 (a) Absorption spectra of **1** measured in a water/MeCN mixture (1/1 v/v; pH 7.4) with Co^{2+} (1 equiv) together with other respective metal cations (1 equiv) after UV irradiation (280 nm) for 1 h. (b) Absorbance of solutions at 472 nm.

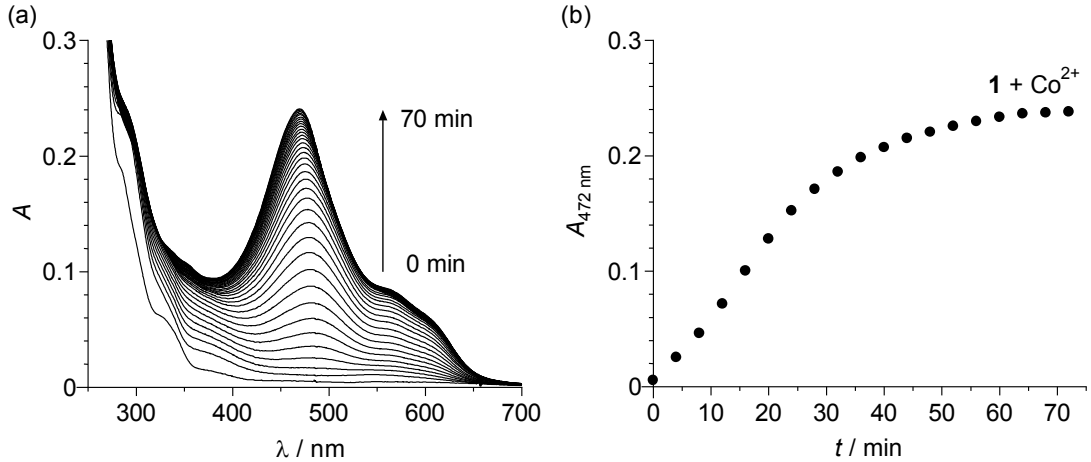


Fig. S9 (a) Time-dependent change in absorption spectra of **1** (20 μM) measured with Co^{2+} (1 equiv) in a water/MeCN mixture (1/1 v/v; pH 7.4) under UV irradiation (280 nm). (b) Change in absorbance at 472 nm.

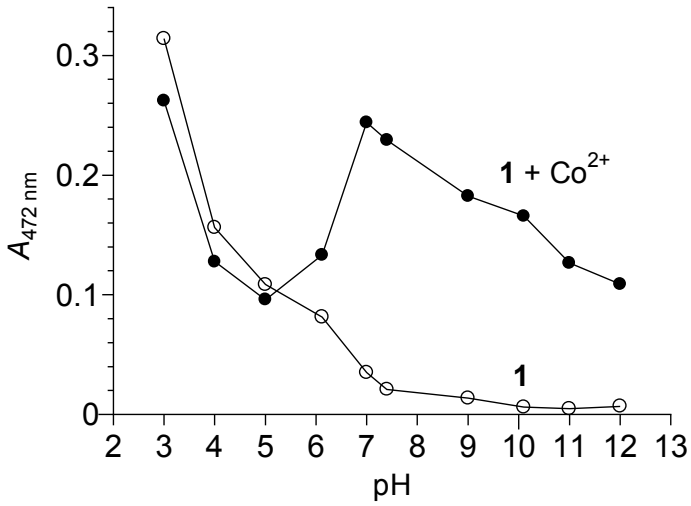


Fig. S10 Effect of pH on the 472 nm absorbance of **1** (20 μM) in a water/MeCN mixture (1/1 v/v; pH 7.4), measured (open) without and (closed) with Co^{2+} (1 equiv) after UV irradiation (280 nm) for 1 h.

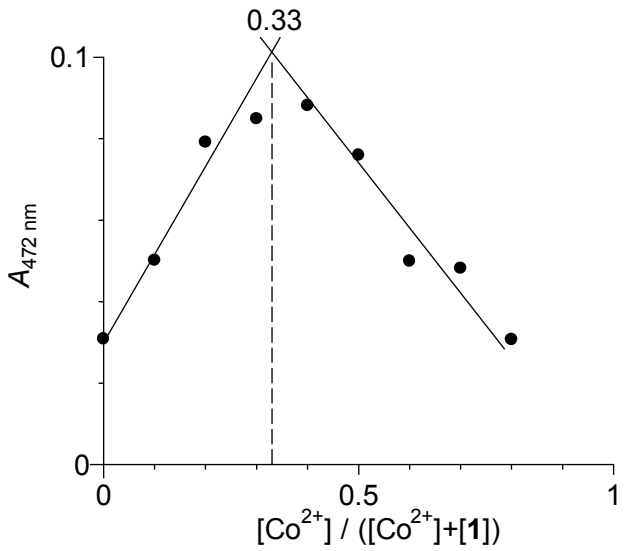
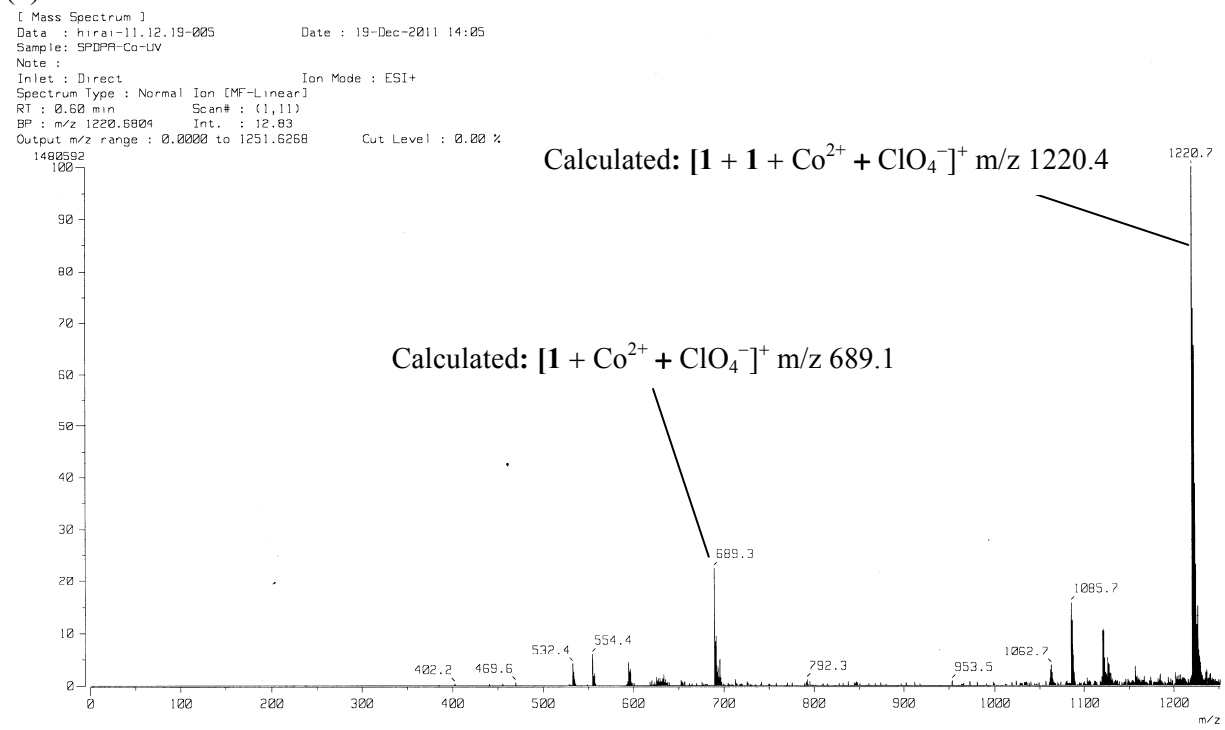


Fig. S11 Job's plot analysis for coloration of **1** with Co^{2+} ([Co^{2+}] + [**1**] = 20 μM). The measurements were carried out in a water/MeCN mixture (1/1 v/v; pH 7.4) after UV irradiation (280 nm) for 1 h.

(a)



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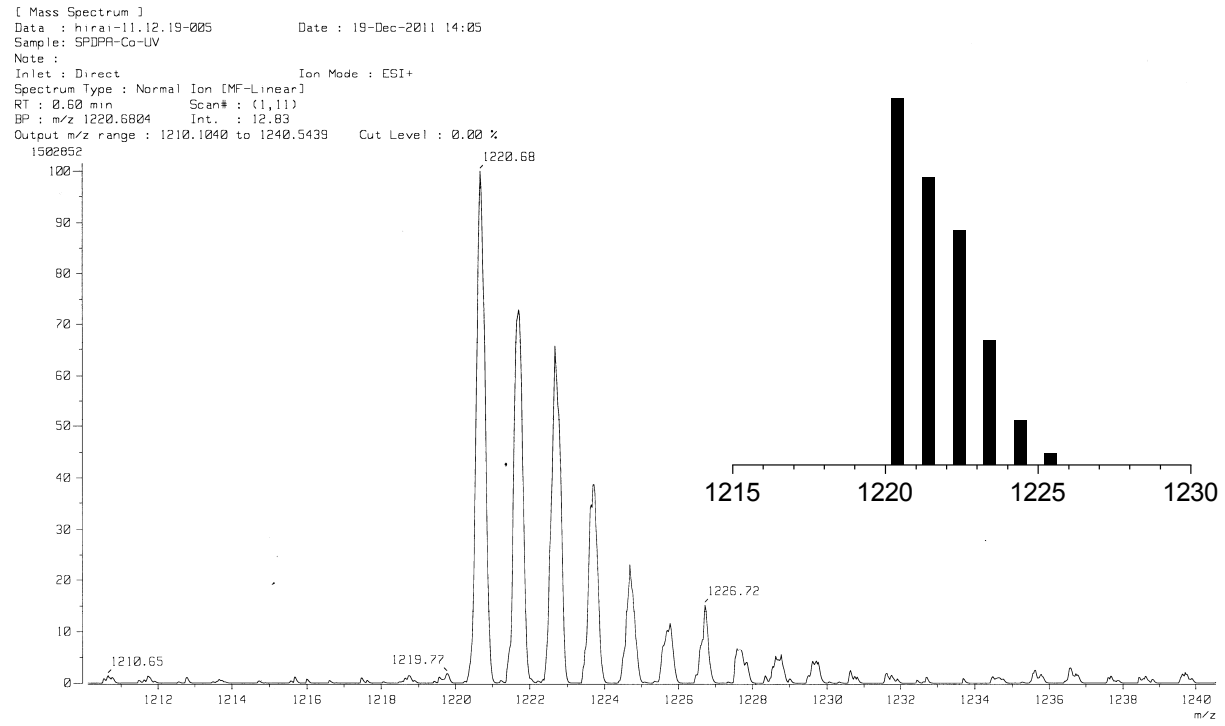
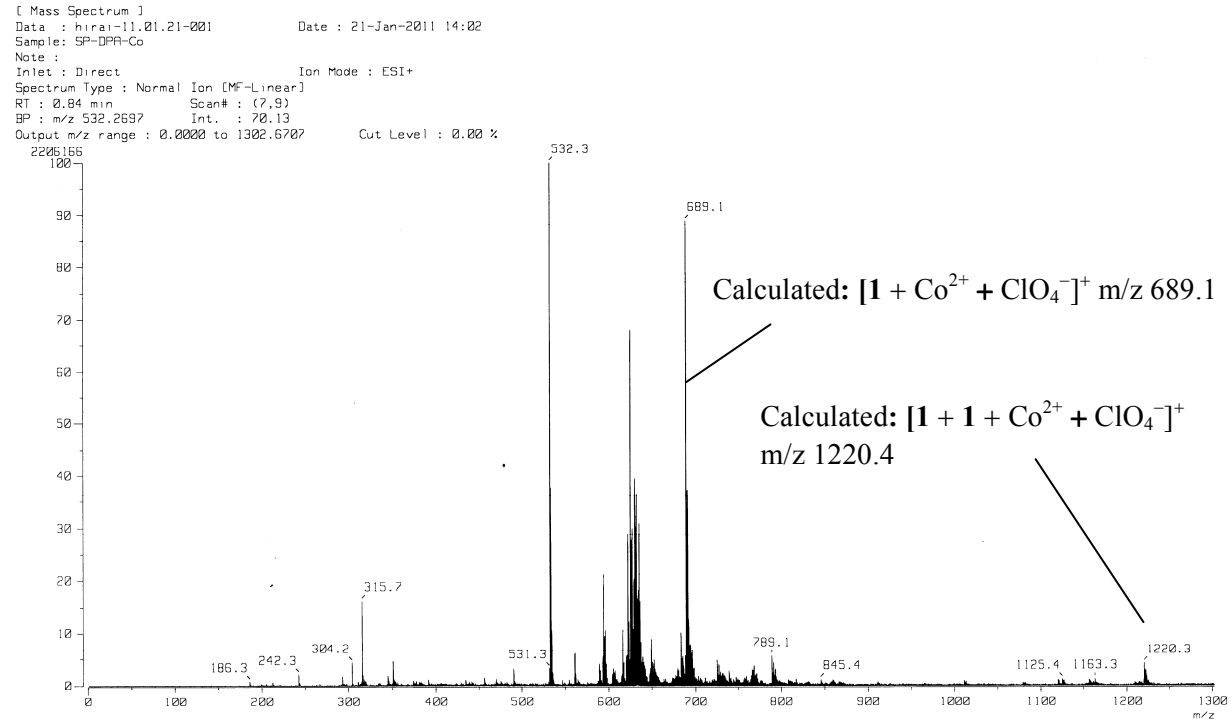


Fig. S12 (a) ESI-MS(+) chart of a water/MeCN (1/1 v/v) solution containing of **1** and 0.5 equiv of $Co(ClO_4)_2$ after UV irradiation for 1 h. (b) Observed isotopic pattern for the [**1** + **1** + Co^{2+} + ClO_4^-]$^+$ signal and the calculated isotopic pattern.

(a)



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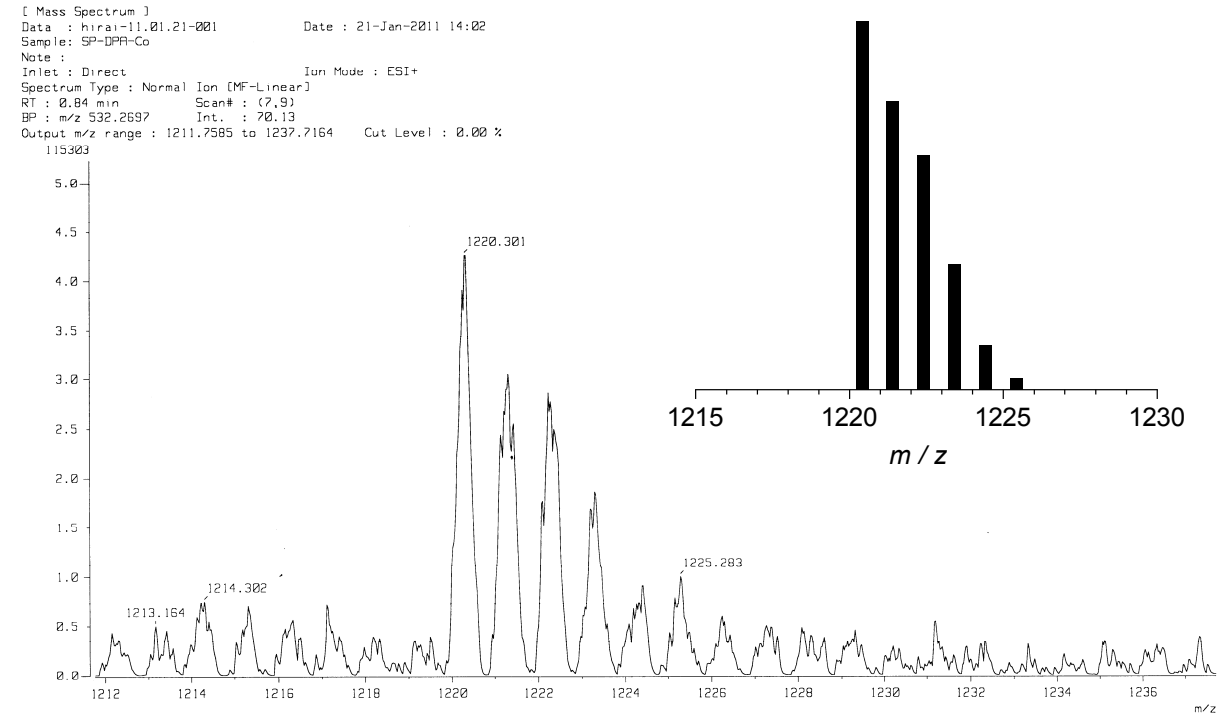
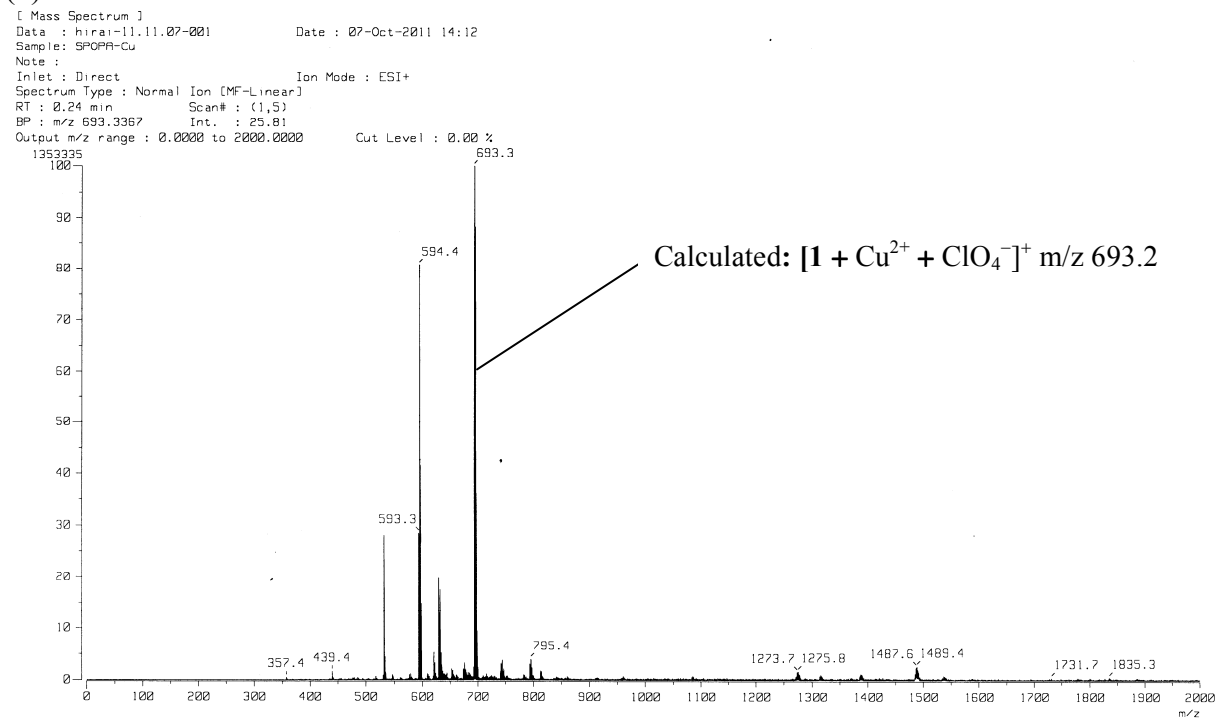


Fig. S13 (a) ESI-MS(+) chart of a water/MeCN (1/1 v/v) solution containing of **1** and 0.5 equiv of $Co(ClO_4)_2$ after treatment in the dark for 1 h. (b) Observed isotopic pattern for the [**1** + **1** + Co^{2+} + ClO_4^-]$^+$ signal and the calculated isotopic pattern.

(a)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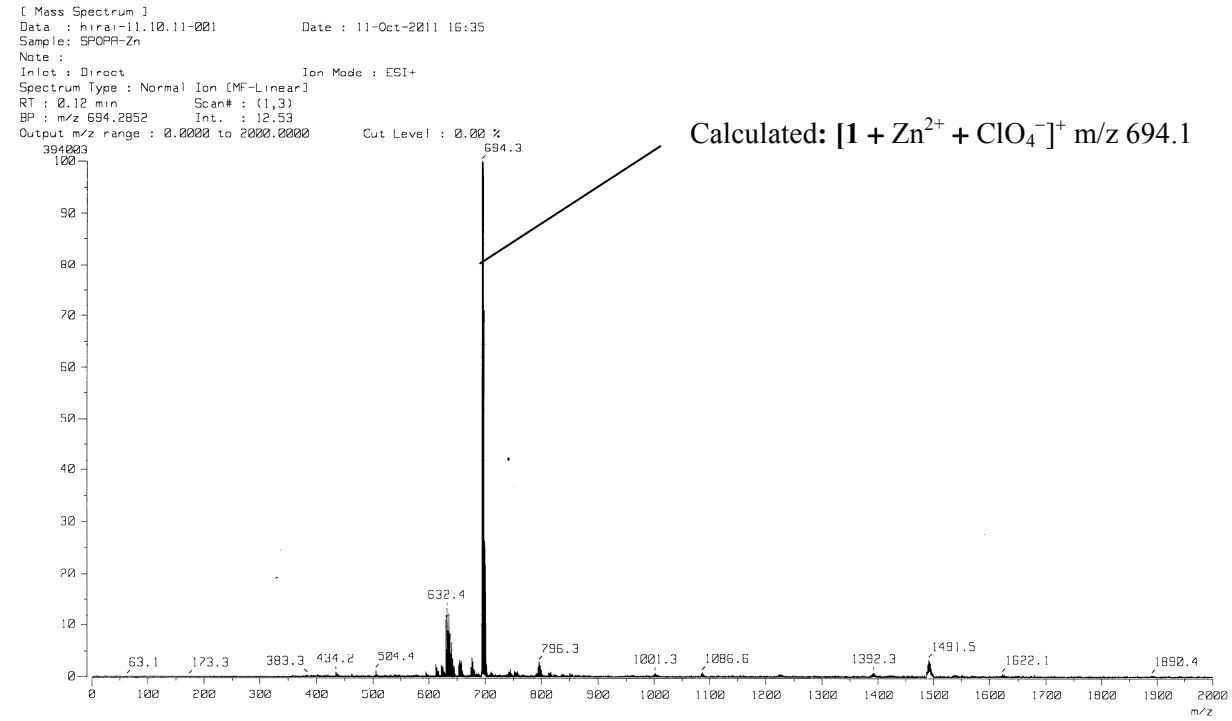
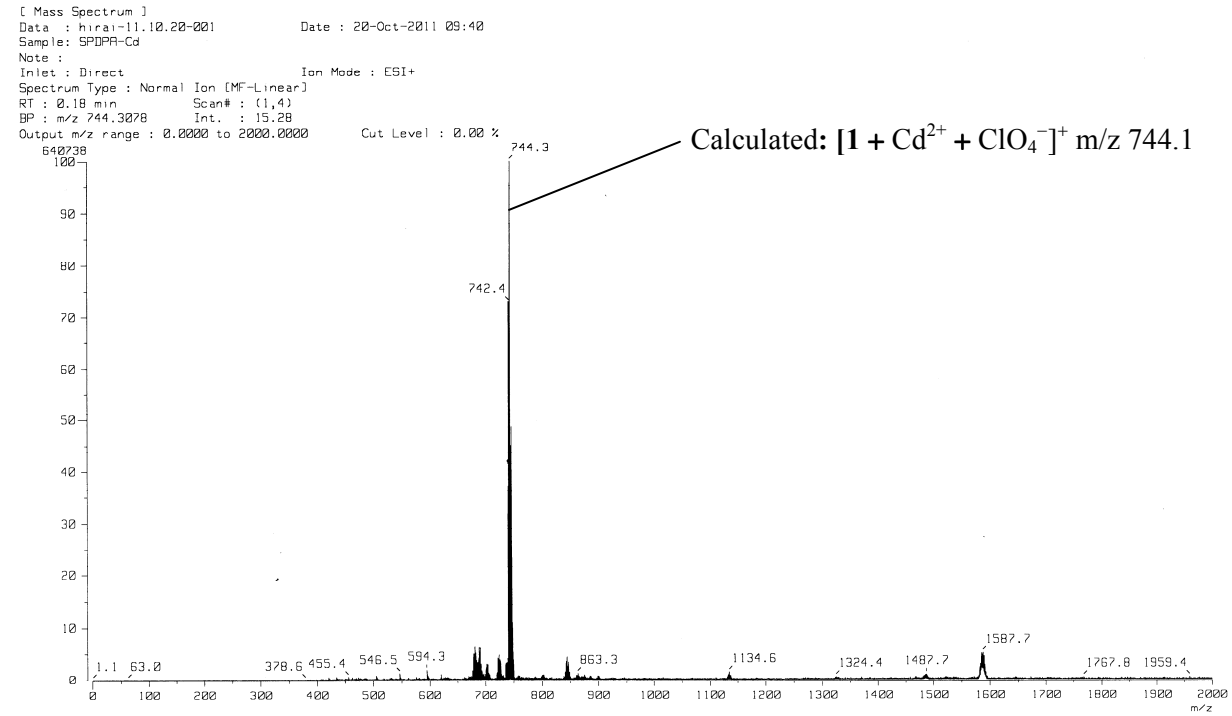
Inlet : Direct Ion Mode : ESI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.24 min Scan# : (1,5)
BP : m/z 693.3367 Int. : 25.81
Output m/z range : 0.0000 to 2000.0000 Cut Level : 0.00 %
1353335
693.3
594.4
593.3
357.4
439.4
795.4
1273.7
1275.8
1487.6
1489.4
1731.7
1835.3
m/z
Calculated: [1 + Cu2+ + ClO4−]+ m/z 693.2

(b)


[Mass Spectrum]
Data : hirai-11.10.11-001 Date : 11-Oct-2011 16:35
Sample: SPOPA-Zn
Note :
Inlet : Direct Ion Mode : ESI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.12 min Scan# : (1,3)
BP : m/z 694.2852 Int. : 12.53
Output m/z range : 0.0000 to 2000.0000 Cut Level : 0.00 %
394003
694.3
632.4
63.1
173.3
383.3
434.2
504.4
796.3
1001.3
1086.6
1392.3
1491.5
1622.1
1890.4
m/z
Calculated: [1 + Zn2+ + ClO4−]+ m/z 694.1

(c)



(d)

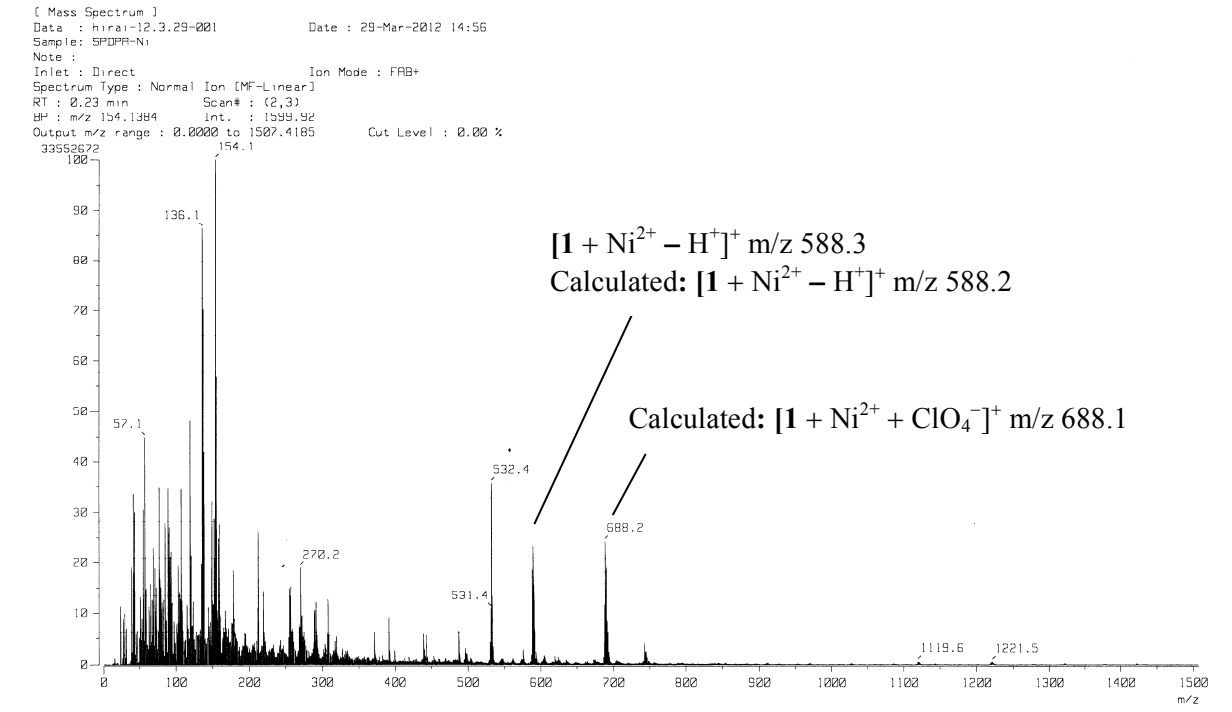


Fig. S14 ESI-MS(+) chart of a solution containing **1** with (a) $Cu(ClO_4)_2$, (b) $Zn(ClO_4)_2$, or (c) $Cd(ClO_4)_2$ (1 equiv) after stirring for 1 h in the dark. (d) FAB-MS chart for **1**(SP)–Ni complex. A solution containing **1** with $Ni(ClO_4)_2$ (1 equiv) was stirred for 1 h in the dark. The solution was concentrated by evaporation, and the resulting solid was used for analysis.

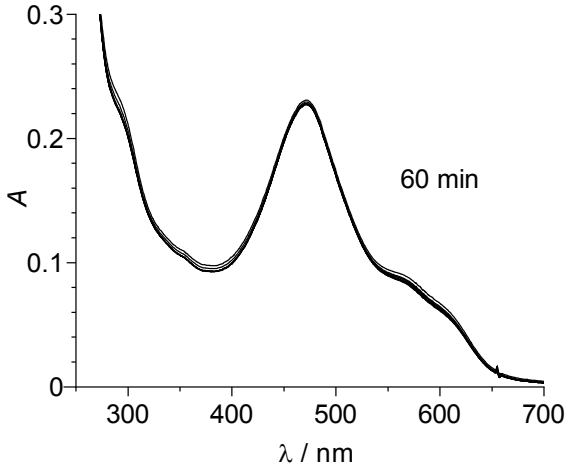


Fig. S15 Time-dependent change in absorption spectra of **1**(MC)–Co^{2+} complex measured in a water/MeCN mixture (1/1 v/v; pH 7.4) under irradiation of visible light (450 nm) for 1 h. The measurements were carried out as follows: UV light (280 nm) was irradiated to the solution containing **1** (20 μM) with Co^{2+} (1 equiv) for 1 h at 25 °C. The spectral measurements were then started under visible light irradiation at 25 °C.

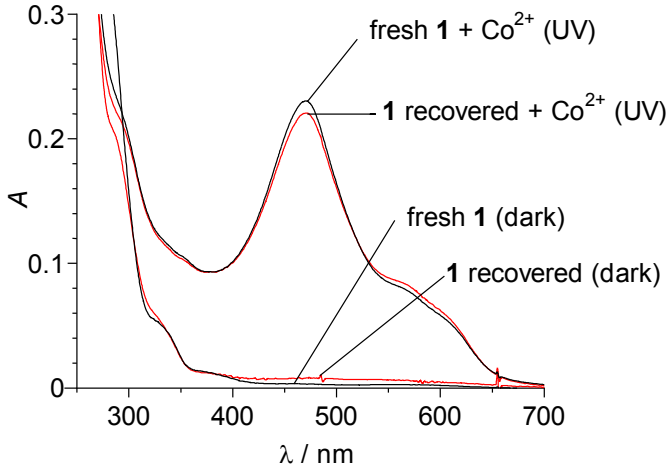
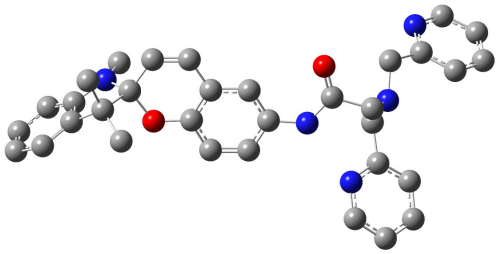


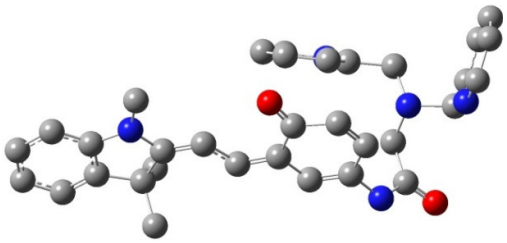
Fig. S16 Absorption spectra of (red) **1** recovered from the solution containing **1**(MC)–Co^{2+} complex. The spectra for fresh **1** are also shown as black lines.
The measurements were carried out as follow:
UV light was irradiated to a water/MeCN mixture (1/1 v/v; pH 7.4) containing **1** with Co^{2+} for 1 h. Excess amount of MeCN was removed by evaporation, and EDTA (5 equiv of Co^{2+}) was added to the resulting solution. The solution was extracted with CH_2Cl_2 and concentrated by evaporation. The resultant was again dissolved in a water/MeCN mixture and spectral measurements were carried out in a similar manner.

Cartesian Coordinates (in Å) of **1**(SP)



C	-8.756111	1.114974	1.383846	C	4.960146	-1.630893	-0.468228	H	-6.998649	-1.988018	-1.499013
C	-8.385195	0.320663	2.473241	C	4.431828	0.497836	0.648779	H	-3.844969	-2.606392	1.441358
C	-7.271601	-0.534442	2.405126	C	4.551547	2.001740	0.565990	H	-5.289308	-2.742026	2.457416
C	-6.548116	-0.573595	1.211788	C	6.278231	-1.965519	0.201260	H	-4.197154	-1.344952	2.647807
C	-6.912511	0.222462	0.108573	C	7.451919	-1.244545	-0.071520	H	-2.260283	-2.592499	-1.957194
C	-8.013095	1.063555	0.187930	C	8.646059	-1.633872	0.540788	H	-4.640341	-2.704915	-1.402580
N	-5.414599	-1.342910	0.897120	C	8.639185	-2.732383	1.409582	H	-2.204582	2.123691	0.947305
C	-4.775161	-0.811660	-0.300005	C	7.429160	-3.395215	1.630549	H	0.228413	2.263988	0.415837
C	-5.977056	-0.086589	-1.057686	N	6.267882	-3.024231	1.046388	H	-0.041012	-1.391387	-1.831460
C	-5.510988	1.149799	-1.842992	C	5.757261	2.661206	0.844264	H	2.079522	1.437390	-0.626056
C	-6.689076	-1.075902	-2.019940	C	5.815295	4.054649	0.757190	H	3.989672	1.291493	-1.922002
C	-4.644870	-2.037910	1.920798	C	4.665509	4.761394	0.385775	H	4.355629	-0.267269	-2.679910
O	-3.835504	0.276649	0.166889	C	3.502762	4.040893	0.107716	H	4.934535	-2.077798	-1.469335
C	-2.485407	0.303821	-0.152525	N	3.440479	2.692106	0.194574	H	4.154951	-2.115584	0.104771
C	-1.885483	-0.698043	-0.936880	O	2.109483	-1.343263	-2.217403	H	5.143042	0.123561	1.391219
C	-2.727559	-1.798489	-1.381384	H	-9.615287	1.773452	1.458961	H	3.420951	0.238871	1.004242
C	-4.039741	-1.860885	-1.085045	H	-8.959535	0.367621	3.393648	H	7.403801	-0.397678	-0.745888
C	-1.723384	1.367716	0.338211	H	-6.984932	-1.135322	3.260987	H	9.566910	-1.094254	0.342466
C	-0.365431	1.438791	0.034161	H	-8.300784	1.681192	-0.658055	H	9.545513	-3.065185	1.903461
C	0.252873	0.449477	-0.759133	H	-4.771626	0.869964	-2.602837	H	7.372673	-4.248904	2.298433
C	-0.515275	-0.622371	-1.237441	H	-5.064734	1.893220	-1.181053	H	6.629925	2.082081	1.124817
N	1.635649	0.605239	-1.030429	H	-6.364282	1.604821	-2.359861	H	6.738458	4.580578	0.976599
C	2.463816	-0.247305	-1.714538	H	-6.039791	-1.349603	-2.859242	H	4.669513	5.842598	0.309897
C	3.929605	0.207421	-1.793145	H	-7.587743	-0.598883	-2.425099	H	2.589904	4.541970	-0.194941
N	4.764153	-0.173573	-0.632111								

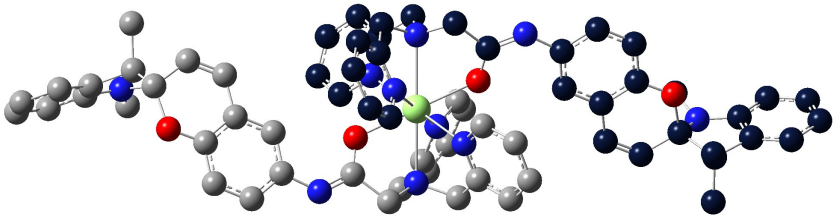
Cartesian Coordinates (in Å) of **1**(MC)



C	-8.667164	0.561277	0.391523	C	3.903477	0.513641	2.089188	H	-3.678710	-3.032314	-0.543119
C	-8.707671	-0.832304	0.401434	C	5.518024	1.017664	0.294313	H	-5.296490	-3.296521	-1.261701
C	-7.550037	-1.600836	0.186224	C	5.977233	-0.379913	-0.066733	H	-5.070827	-3.403121	0.518134
C	-6.362989	-0.912247	-0.035918	C	6.636657	-1.195470	0.876126	H	-2.449857	-1.658875	-0.803559
C	-6.308651	0.513476	-0.050441	C	7.051723	-2.471052	0.489969	H	-2.167110	1.434996	-0.912096

C	-7.457711	1.248191	0.163628	C	6.811201	-2.908143	-0.816202	H	1.912185	-2.307622	-1.761201
N	-5.054153	-1.426113	-0.263716	C	6.158262	-2.037413	-1.702310	H	3.371050	-0.268823	-2.045013
C	-4.126895	-0.389514	-0.473041	N	5.747302	-0.792929	-1.344132	H	-0.033653	2.294205	-1.307127
C	-4.877633	0.963844	-0.320768	O	4.330619	3.551095	-1.356570	H	2.711257	2.530595	-2.889440
C	-4.321888	1.742545	0.872255	C	1.765451	-0.804642	1.658705	H	2.328311	2.184672	0.772339
C	-4.796555	1.763532	-1.621205	C	2.453464	0.190428	2.376001	H	3.825472	3.101264	1.109967
C	-4.766433	-2.862837	-0.395437	N	1.870907	0.898286	3.385473	H	4.287719	1.255947	2.828275
C	-2.811404	-0.612210	-0.740273	C	0.580065	0.614405	3.701290	H	4.501779	-0.417823	2.230510
C	-1.820672	0.389045	-0.952599	C	-0.170626	-0.362005	3.028352	H	6.164522	1.449404	1.088960
C	-0.493489	0.159646	-1.208181	C	0.436288	-1.074824	1.989077	H	5.658930	1.685413	-0.596010
C	0.096740	-1.199554	-1.290524	H	-9.578315	1.131418	0.560969	H	6.823045	-0.836092	1.884451
C	1.526607	-1.294060	-1.658745	H	-9.653929	-1.344533	0.579013	H	7.560886	-3.121128	1.201675
C	2.298213	-0.204452	-1.825446	H	-7.592014	-2.684708	0.195601	H	7.123045	-3.896827	-1.141176
C	1.710222	1.125753	-1.691484	H	-7.437513	2.336233	0.157358	H	5.951722	-2.328429	-2.739089
C	0.394794	1.294520	-1.401568	H	-3.266521	2.006850	0.734772	H	2.265339	-1.334063	0.845924
O	-0.537474	-2.219633	-1.042021	H	-4.394487	1.160577	1.800568	H	0.150287	1.199658	4.521498
N	2.558620	2.274941	-1.908392	H	-4.878448	2.674225	1.029928	H	-1.201632	-0.558087	3.307759
C	3.502119	2.733708	-0.981804	H	-3.765887	2.055878	-1.858102	H	-0.124555	-1.831358	1.431173
C	3.399402	2.290876	0.473192	H	-5.394449	2.680793	-1.559636				
N	4.063033	0.962176	0.663536	H	-5.177010	1.185526	-2.473844				

Cartesian Coordinates (in Å) of 2:1 **1**(SP)–Co^{2+} complex



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N	3.428059	-0.585424	2.883629	H	-1.125469	-0.561588	-4.010524	H	-3.372182	4.278820	0.008532
C	2.209648	-0.337600	2.383547	H	-0.525838	-1.761351	-2.840428	H	5.715320	0.855095	-1.550393
C	1.013981	-0.685095	3.257174	H	-3.301783	-1.138612	-3.512177	H	14.480639	0.973855	0.675256
O	1.985065	0.147873	1.209721	H	-1.075882	1.794577	-2.630765	C	4.950764	-0.006587	0.933513
N	-0.135721	0.098891	2.762373	H	0.180728	1.788050	-3.884981	C	5.842550	-0.786219	3.040101
H	1.231918	-0.508424	4.322257	C	2.108717	4.483483	-1.595949	H	7.992709	-0.975715	3.151057
H	0.775417	-1.746809	3.127687	H	1.075234	4.006730	-3.432206	C	4.734648	-0.440286	2.246204
Co	0.054938	0.106936	0.165506	H	3.063727	4.578230	0.343680	H	4.105794	0.277627	0.320352
C	-0.042891	1.530363	3.149486	H	3.084978	-4.364248	0.304897	H	5.715080	-1.122210	4.066345
C	-1.445352	-0.503979	3.102444	C	3.383739	-3.419039	-1.620436	H	-8.723863	-2.730738	0.621356
N	-1.088734	-1.804974	1.051057	H	3.392309	-2.232877	-3.422886	C	-9.696910	-2.478697	0.183375
N	-1.197981	1.901037	1.031942	H	2.262029	0.509675	-2.622788	C	-10.182219	-1.112755	0.684839
O	-1.867554	-0.036755	-0.863889	H	1.659856	-0.562109	-3.901800	H	-9.602465	-2.497505	-0.903862
N	1.121477	2.016666	-0.704723	H	-2.910426	5.140777	2.320322	H	-10.406016	-3.259185	0.482648
N	1.392212	-1.636169	-0.769817	H	-3.612919	-4.539090	2.173609	C	-11.453743	-0.611995	0.017914
C	-0.973924	2.353147	2.289471	H	2.487614	5.436213	-1.944254	C	-9.174243	0.057737	0.310725
H	0.989539	1.849604	2.973220	H	4.153949	-4.103637	-1.952618	C	-10.415205	-1.177984	2.212701

H	-0.271281	1.688743	4.214385	H	9.955786	-3.169088	-1.259826	C	-11.319800	0.762837	-0.233302
C	-1.711506	-1.725276	2.250570	C	9.350980	-2.386739	-0.786955	C	-12.634607	-1.266530	-0.291725
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H	-1.525994	-0.758397	4.169986	H	8.312978	-2.531497	-1.109098	O	-8.645711	-0.238282	-1.023562
C	-1.377896	-2.868649	0.254885	H	9.399425	-2.520607	0.295215	C	-8.077326	0.306780	1.307256
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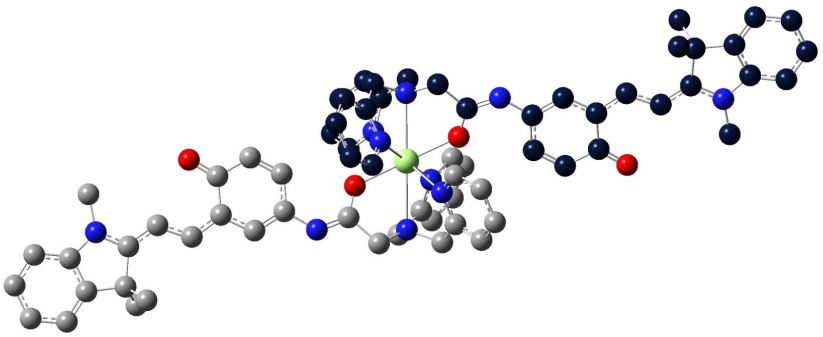
C	1.924180	2.778101	0.081724	C	11.246072	0.688503	-0.270650	C	-12.359398	1.495874	-0.803448
C	1.807126	-2.663832	0.018282	C	12.405940	-1.407891	-0.602774	C	-13.693310	-0.542470	-0.863830
C	1.974843	-1.497132	-1.984416	N	9.976571	1.252587	-0.455562	H	-12.742830	-2.331889	-0.101231
C	-1.575730	3.511040	2.782083	O	8.633668	-0.236840	0.776605	C	-9.523689	2.467139	-0.317373
C	-2.614495	-2.699382	2.685113	C	7.804400	0.595854	-1.384848	C	-7.314640	-0.337042	-1.300562
C	-2.274089	-3.865545	0.615579	H	8.904070	-1.131174	-3.182746	C	-6.772638	0.203762	1.012804
H	-0.852857	-2.907206	-0.688144	H	10.599544	-1.646090	-3.147232	H	-8.476425	-0.107933	2.226274
C	-2.688794	3.763531	0.670488	H	10.208000	0.077666	-3.093165	C	-13.549704	0.822295	-1.111220
H	-2.265337	2.163509	-0.715973	C	12.402233	1.291917	0.221578	H	-12.255692	2.555791	-1.014336
C	-0.866007	-0.725477	-2.952425	C	13.580619	-0.814681	-0.112197	H	-14.621650	-1.047214	-1.115863
N	-3.273949	-0.827801	-2.540732	H	12.410339	-2.449967	-0.914232	H	-8.540687	2.637242	0.128648
C	-0.019378	1.579808	-2.822687	C	9.605464	2.474558	0.235423	H	-10.179474	3.290561	-0.015840
C	1.315652	3.690784	-2.424547	C	7.347056	-0.288104	1.224069	H	-9.421866	2.480062	-1.412592
C	2.425854	4.011104	-0.321322	C	6.545867	0.536885	-0.924270	C	-6.323333	-0.143453	-0.324960
H	2.182338	2.348258	1.035269	H	8.017898	0.974179	-2.378391	C	-6.949518	-0.636407	-2.614128
C	2.791031	-3.565496	-0.363083	C	13.570521	0.520191	0.290798	H	-6.019902	0.395094	1.774298
H	1.309804	-2.754257	0.972497	H	12.404617	2.326073	0.551937	H	-14.369724	1.377848	-1.559397
C	2.961223	-2.376541	-2.439728	H	14.494866	-1.397480	-0.044279	C	-4.969562	-0.261747	-0.667471
C	1.569696	-0.312449	-2.833728	H	8.587270	2.750080	-0.050161	C	-5.604290	-0.755233	-2.946599
C	-2.434621	4.237881	1.958473	H	10.273976	3.286803	-0.068493	H	-7.725584	-0.775471	-3.360139
H	-1.379023	3.828481	3.798716	H	9.650001	2.371682	1.329710	C	-4.599009	-0.573683	-1.980232
C	-2.908501	-3.779753	1.858219	C	6.252621	0.070013	0.420357	H	-4.202758	-0.103862	0.079374
H	-3.082122	-2.600138	3.656977	C	7.137339	-0.709716	2.538076	H	-5.324281	-0.987347	-3.971310

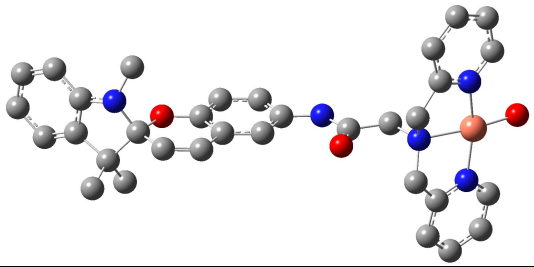
Cartesian Coordinates (in Å) of 2:1 **1**(MC)–Co^{2+} complex



C	15.536276	-2.055122	0.874253	C	-0.418836	-0.500229	3.260895	H	3.009868	5.162654	0.110557
C	15.781220	-1.482844	-0.377245	N	-0.827325	-1.396281	1.011836	H	2.782033	-3.638691	-1.551227
C	14.741132	-0.930932	-1.134556	N	-0.838842	2.235466	1.693618	C	2.456631	-2.340646	-3.253689
C	13.460156	-0.973089	-0.597071	O	-2.165185	0.650019	-0.186947	H	1.902876	-0.841355	-4.703448

C	13.201603	-1.544088	0.655806	N	0.761508	2.759012	-0.663156	H	1.161888	1.657458	-3.082789
C	14.236104	-2.088076	1.399762	N	0.897340	-0.827267	-1.481038	H	0.136822	0.817013	-4.262197
N	12.234146	-0.496953	-1.137796	C	-0.183116	2.469881	2.856332	H	-1.921438	5.132862	4.043263
C	11.184442	-0.730097	-0.301600	H	1.882834	1.928547	2.726275	H	-2.894095	-4.373501	2.416081
C	11.710677	-1.438276	0.964198	H	1.120883	1.506287	4.274282	H	1.724326	6.387421	-1.664189
C	11.491253	-0.565147	2.228425	C	-0.998827	-1.555488	2.345373	H	3.059229	-2.920687	-3.941217
C	11.095493	-2.854993	1.110149	H	-1.194319	0.248271	3.454796	H	-6.614844	-0.201273	-1.838011
C	12.106231	0.168725	-2.448698	H	-0.133016	-0.947107	4.225044	C	-6.365307	-0.185063	-0.778389
C	9.888713	-0.350597	-0.641731	C	-1.402262	-2.309512	0.184245	C	-7.424517	-0.347979	0.152287
C	8.748096	-0.530555	0.134424	C	-1.903756	3.020873	1.392785	C	-5.055465	-0.011436	-0.389324
C	7.444019	-0.140146	-0.236190	C	-2.752144	0.399709	-1.289905	C	-8.736087	-0.510858	-0.341419
C	7.158334	0.516283	-1.531823	C	0.088967	3.412565	-1.641492	C	-7.126139	-0.339431	1.602062
C	5.755892	0.854249	-1.749667	C	1.800997	3.397974	-0.068877	C	-4.736414	0.009762	1.008076
C	4.767142	0.595809	-0.852791	C	1.522223	-1.966128	-1.079221	C	-9.871633	-0.682714	0.443594
C	5.074954	-0.042734	0.392989	C	1.052754	-0.442260	-2.769748	H	-8.839222	-0.494766	-1.423809
C	6.379127	-0.389408	0.668600	C	-0.549300	3.500539	3.721802	C	-5.719059	-0.145995	1.934936
O	8.035412	0.778564	-2.405320	C	-1.727005	-2.622391	2.878921	O	-7.996824	-0.484213	2.508749
H	16.356533	-2.475920	1.442052	C	-2.149508	-3.385471	0.643342	H	-3.708801	0.158572	1.298868
H	16.789652	-1.463829	-0.771513	H	-1.232194	-2.160524	-0.871841	C	-11.176315	-0.836638	-0.017623
H	14.944869	-0.492057	-2.102167	C	-2.317484	4.072948	2.202807	H	-9.685333	-0.689996	1.510914
H	14.051305	-2.532871	2.370775	H	-2.437976	2.756388	0.495596	H	-5.490495	-0.129503	2.993365
H	10.426477	-0.448737	2.447282	C	-1.925412	0.381389	-2.575175	N	-12.218279	-0.997514	0.844730
H	11.933220	0.425015	2.088052	N	-4.058809	0.123197	-1.407228	C	-11.723144	-0.857265	-1.460196
H	11.975281	-1.045268	3.085075	C	-1.032244	2.657421	-2.318531	C	-13.457324	-1.136448	0.161077
H	10.018085	-2.799365	1.286672	C	0.412784	4.713867	-2.025163	C	-12.071175	-1.023143	2.312998
H	11.564729	-3.365936	1.957123	C	2.171335	4.699085	-0.392148	C	-13.215958	-1.060866	-1.216873
H	11.275331	-3.442114	0.205447	H	2.352915	2.817812	0.651863	C	-11.481790	0.502742	-2.167775
H	11.456346	-0.416580	-3.105294	C	2.305047	-2.741598	-1.923167	C	-11.146721	-2.052505	-2.264544
H	13.093721	0.253389	-2.899046	H	1.362482	-2.250514	-0.049767	C	-14.735790	-1.320057	0.674242
H	11.679456	1.167319	-2.320865	C	1.814213	-1.181787	-3.679087	H	-11.423750	-1.852655	2.610699
H	9.712919	0.132928	-1.595320	C	0.417973	0.862078	-3.199135	H	-13.053813	-1.151952	2.763492
H	8.840731	-1.005154	1.108378	C	-1.622116	4.325737	3.386358	H	-11.632491	-0.084158	2.661747
H	5.536544	1.339867	-2.692433	H	-0.005930	3.643807	4.647660	C	-14.266184	-1.169581	-2.114045
H	3.742423	0.866358	-1.051069	C	-2.317984	-3.545955	2.021697	H	-10.414274	0.684956	-2.317668
H	6.619423	-0.875448	1.612767	H	-1.830231	-2.715789	3.953030	H	-11.899555	1.319600	-1.572999
H	4.427812	-0.853143	2.179689	H	-2.586813	-4.082966	-0.058748	H	-11.977291	0.493138	-3.143906
N	4.072628	-0.348676	1.366919	H	-3.175211	4.668321	1.918989	H	-10.069260	-1.943587	-2.414180
C	2.763108	-0.062642	1.364690	N	-0.725963	1.204691	-2.324831	H	-11.634315	-2.095913	-3.243827
C	1.937681	-0.614259	2.526912	H	-2.513113	0.721918	-3.442391	H	-11.336926	-2.992104	-1.738696
O	2.170645	0.607224	0.456491	H	-1.591957	-0.644517	-2.768333	C	-15.791738	-1.428830	-0.238353
N	0.709120	0.201088	2.606241	H	-4.414652	-0.007754	-2.354492	H	-14.925771	-1.379280	1.737658
H	2.512813	-0.622709	3.466257	H	-1.957049	2.794333	-1.748345	C	-15.564242	-1.355159	-1.615518
H	1.641567	-1.644050	2.297224	H	-1.196923	3.054000	-3.332113	H	-14.095373	-1.113621	-3.182900
Co	-0.001703	0.683843	0.146405	C	1.458524	5.376061	-1.383032	H	-16.798777	-1.572232	0.133203
C	0.965900	1.544866	3.185326	H	-0.142712	5.192843	-2.822007	H	-16.396573	-1.442057	-2.302525

Cartesian Coordinates (in Å) of 1:1 **1**(SP)–Cu^{2+} complex



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C	1.590803	0.010950	0.060385	H	3.661701	4.031657	1.570114	H	-5.860081	-2.142349	-1.212857
C	3.045261	0.021137	-0.474826	H	5.082413	5.714597	0.393288	H	-6.910090	-3.230450	-0.270832
N	4.063616	-0.006516	0.628758	H	6.948820	4.933713	-1.079482	H	-6.502706	-2.099174	2.515594
C	3.994727	-1.300065	1.412835	H	7.307490	2.408987	-1.316969	H	-8.111991	-2.350180	1.803038
C	4.000592	1.249742	1.471372	H	3.633201	-4.080917	1.377926	H	-7.686959	-0.758318	2.459980
C	4.754985	2.364684	0.766322	H	7.290638	-2.350381	-1.430806	O	-4.940603	-0.024030	-0.642593
C	4.480645	3.718205	0.935404	H	6.913018	-4.880641	-1.313343	C	-4.864500	-0.033958	1.851426
C	5.279578	4.656525	0.272393	H	5.040595	-5.716611	0.121126	H	-5.167714	2.513335	1.266672
C	6.323981	4.225743	-0.552136	H	-10.842988	-0.641593	-1.947788	H	-6.758012	3.224199	0.934815
C	6.544903	2.859777	-0.692906	C	-9.986594	-0.229535	-1.428296	H	-5.683577	2.782112	-0.422101
N	5.771363	1.965737	-0.036120	C	-9.843179	1.152388	-1.305852	C	-3.570859	0.002478	-0.650832
O	1.357428	-0.018597	1.290842	C	-9.019838	-1.090080	-0.878932	H	-5.386718	-0.016172	2.798596
C	4.454585	-3.743842	0.758664	C	-8.739353	1.711474	-0.644120	C	-3.524996	-0.047899	1.796515
C	4.739507	-2.386017	0.654470	H	-10.590530	1.810553	-1.733740	C	-2.805937	-0.027236	0.529975
N	5.758512	-1.956942	-0.128994	H	-9.130709	-2.164742	-0.973041	C	-2.922877	0.055164	-1.890147
C	6.525033	-2.824482	-0.828088	C	-7.929341	-0.545731	-0.225030	H	-2.939384	-0.055874	2.710196
C	6.293774	-4.193924	-0.752361	C	-7.790982	0.848004	-0.105063	C	-1.409318	-0.015138	0.462071
C	5.246106	-4.655548	0.051085	H	-8.633453	2.786044	-0.566684	C	-1.537077	0.064534	-1.952523
Cu	5.950733	0.008491	-0.281210	C	-6.781627	-1.221087	0.521769	H	-3.525133	0.081301	-2.787791
H	0.982169	0.059789	-1.885512	N	-6.609995	1.154028	0.605389	H	-0.816982	-0.037672	1.363403
H	3.219585	0.923129	-1.071442	C	-6.169818	-2.425733	-0.207049	C	-0.766798	0.027498	-0.778477
H	3.216161	-0.852933	-1.112498	C	-7.297413	-1.629639	1.924645	H	-1.049604	0.098832	-2.921662
H	2.957698	-1.564359	1.622811	C	-5.754484	-0.017420	0.642985	O	7.466261	0.029518	-1.363791
H	4.506971	-1.124702	2.366366	C	-6.020401	2.497051	0.583512	H	8.317274	0.012440	-0.844035
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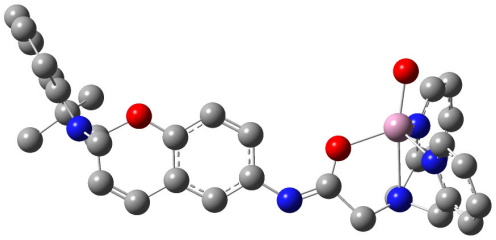
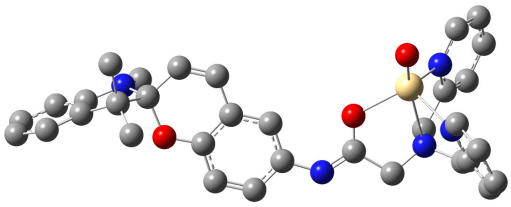
Cartesian Coordinates (in Å) of 1:1 **1**(SP)–Zn^{2+} complex



N	0.837473	-0.530677	-1.756287	H	6.477514	-0.004391	-1.078731	C	-5.654094	-0.139631	-0.786174
C	2.003718	-0.432976	-1.106366	H	5.957083	-1.070829	-2.402569	C	-5.837830	-2.574506	-0.115902
C	3.270638	-0.741428	-1.925147	H	6.952379	-3.188111	-1.597337	H	-5.170141	2.618910	-1.253808

N	4.408912	0.004909	-1.337760	H	6.991969	-4.979565	0.141827	H	-5.114349	2.319608	0.501953
C	4.502459	1.421626	-1.803055	H	5.758669	-4.616359	2.292908	H	-6.454722	3.254321	-0.207070
C	5.708035	-0.721527	-1.390900	H	4.515399	-2.444421	2.603057	H	-7.073618	1.571052	-2.650187
C	5.719946	-1.885469	-0.411849	H	5.938635	3.809181	-1.975167	H	-8.312901	2.051453	-1.470669
C	6.426075	-3.060303	-0.659899	H	4.789075	2.304199	2.570870	H	-8.129784	0.338954	-1.893107
C	6.447705	-4.059831	0.316718	H	6.004480	4.564645	2.272733	O	-4.418114	0.088613	0.081088
C	5.760218	-3.862909	1.517081	H	6.583327	5.270744	-0.057674	C	-5.270574	-0.424321	-2.208603
C	5.068056	-2.670009	1.698916	H	-9.477782	1.287591	3.257622	H	-5.279659	-2.769842	-1.034636
N	5.047495	-1.706247	0.748261	C	-8.856183	0.730900	2.567198	H	-6.645979	-3.307753	-0.041552
O	2.100759	-0.151994	0.129286	C	-8.740909	-0.653465	2.692581	H	-5.167870	-2.688915	0.746671
C	5.703877	3.521807	-0.957972	C	-8.165583	1.406668	1.545872	C	-3.145817	-0.083794	-0.385162
C	5.029153	2.331304	-0.700572	C	-7.936240	-1.396649	1.815566	H	-6.103977	-0.569982	-2.882482
N	4.745527	1.956408	0.561206	H	-9.274034	-1.168073	3.483538	C	-4.005368	-0.528679	-2.639339
C	5.085900	2.735514	1.616950	H	-8.255831	2.482738	1.446558	C	-2.872459	-0.375313	-1.737498
C	5.743414	3.946503	1.424442	C	-7.371333	0.679989	0.677322	C	-2.085872	0.047475	0.519725
C	6.061543	4.338394	0.120409	C	-7.259651	-0.714478	0.809810	H	-3.799911	-0.747883	-3.682343
Zn	3.908501	0.087516	1.067678	H	-7.845866	-2.469300	1.930201	C	-1.547428	-0.517042	-2.150716
H	0.878506	-0.749548	-2.750983	C	-6.585723	1.123737	-0.554560	C	-0.768902	-0.090985	0.103851
H	3.122754	-0.532069	-2.993632	N	-6.407366	-1.225005	-0.193733	H	-2.317712	0.268725	1.552556
H	3.480186	-1.811909	-1.810637	C	-5.772506	2.411566	-0.361783	H	-1.346810	-0.741195	-3.194892
H	3.484042	1.747862	-2.048482	C	-7.586668	1.274616	-1.728228	C	-0.491992	-0.375250	-1.244175
H	5.115031	1.517425	-2.709971	H	4.480084	-0.089458	3.513167	H	0.041627	0.022466	0.804434
O	3.825759	0.367049	2.925180								

Cartesian Coordinates (in Å) of 1:1 **1**(SP)–Cd^{2+} complex



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C	-2.944488	-0.607476	2.092201	H	-7.170796	-4.720415	0.693909	H	6.737556	-3.106224	-1.023418
N	-4.051636	0.138676	1.446861	H	-6.168284	-4.624630	-1.596475	H	5.820981	-1.153107	-3.157307
C	-4.012627	1.603386	1.730510	H	-4.750727	-2.554043	-2.199550	H	7.530819	-1.550904	-2.879153
C	-5.389981	-0.478601	1.712353	H	-5.583618	3.827698	2.041853	H	7.021261	0.147689	-2.887777
C	-5.605982	-1.721140	0.857551	H	-5.055142	2.392804	-2.622083	O	4.921023	-0.296169	0.738158
C	-6.368361	-2.807883	1.279665	H	-6.378293	4.456848	-2.146661	C	4.377097	0.504343	-1.563829
C	-6.578107	-3.866659	0.388729	H	-6.652459	5.182807	0.238400	H	4.821840	2.731381	-0.246943
C	-6.017823	-3.818550	-0.891026	H	10.967278	-1.007239	0.629017	H	6.458066	3.378854	-0.028943
C	-5.250710	-2.711177	-1.245599	C	10.031888	-0.492712	0.446538	H	5.672359	2.488971	1.305278
N	-5.061712	-1.691409	-0.373922	C	9.888929	0.845530	0.812466	C	3.583841	-0.311189	1.014820
O	-1.622778	0.008589	0.129077	C	8.963055	-1.176930	-0.158520	H	4.708467	0.841892	-2.536598
C	-5.481738	3.541738	1.002706	C	8.685112	1.532511	0.593497	C	3.072714	0.423072	-1.265784
C	-4.744465	2.408359	0.664957	H	10.716049	1.366340	1.280728	C	2.607667	0.014588	0.052588
N	-4.606530	2.020216	-0.627200	H	9.074414	-2.217028	-0.444381	C	3.182397	-0.673053	2.307513

C	-5.190399	2.750369	-1.608930	C	7.773676	-0.505595	-0.377790	H	2.324848	0.683269	-2.007923
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C	-6.078087	4.298651	-0.008471	H	8.582504	2.567918	0.892266	C	1.835597	-0.726958	2.630002
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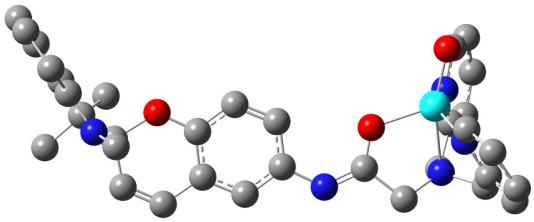
H	-0.634305	-0.752007	3.063251	N	6.344036	1.303360	-0.340005	H	0.503350	0.203823	-0.354136
H	-2.851863	-0.387923	3.166605	C	6.012707	-2.361363	-0.678010	C	0.857276	-0.415696	1.670366
H	-3.167336	-1.675265	1.974826	C	6.722689	-0.866249	-2.604422	H	1.541475	-1.019080	3.633041
H	-2.957830	1.902739	1.713870	C	5.482197	0.171507	-0.605036	H	-2.637675	-1.169230	-3.226719
H	-4.419520	1.844039	2.722670	C	5.794172	2.544694	0.215284	O	-3.537439	-0.895896	-2.902866
H	-6.139958	0.269067	1.428469								

Cartesian Coordinates (in Å) of 1:1 **1**(SP)–Ni^{2+} complex



N	0.941949	-0.593489	-1.688002	H	6.556022	-0.037200	-0.799497	H	-5.044889	2.454916	-1.474877
C	2.102215	-0.448685	-1.032522	H	6.108102	-1.035383	-2.208225	H	-5.014699	2.310673	0.301437
C	3.384985	-0.774367	-1.809729	H	7.120496	-3.165173	-1.339624	H	-6.336732	3.189628	-0.506125
N	4.500967	0.008104	-1.194762	H	6.933940	-5.048272	0.291491	H	-6.937880	1.293607	-2.799102
C	4.588936	1.400686	-1.760556	H	5.379439	-4.814395	2.243055	H	-8.186083	1.898853	-1.687734
C	5.804356	-0.730024	-1.197690	H	4.075905	-2.692216	2.487217	H	-8.021857	0.152279	-1.946337
C	5.708367	-1.939461	-0.279042	H	5.730829	3.920447	-2.002232	O	-4.333060	0.039871	0.089341
C	6.460672	-3.093164	-0.484149	H	4.496353	2.571264	2.562962	C	-5.165891	-0.662567	-2.157073
C	6.353782	-4.144510	0.429825	H	5.407978	4.931695	2.178035	H	-5.221540	-2.900470	-0.781717
C	5.488243	-4.018551	1.518664	H	6.047704	5.572793	-0.157076	H	-6.586798	-3.324653	0.266385
C	4.758511	-2.841996	1.661144	H	-9.405064	1.573691	3.090660	H	-5.098735	-2.644061	0.982069
N	4.865137	-1.821667	0.778424	C	-8.783940	0.950921	2.458709	C	-3.055178	-0.135566	-0.361983
O	2.197841	-0.107106	0.187062	C	-8.682159	-0.417043	2.711028	H	-5.993841	-0.885984	-2.816086
C	5.449568	3.675771	-0.985392	C	-8.080598	1.524302	1.384851	C	-3.897312	-0.780873	-2.573534
C	4.898504	2.431475	-0.687149	C	-7.878773	-1.244394	1.911689	C	-2.771107	-0.525556	-1.686532
N	4.555085	2.100475	0.573245	H	-9.225238	-0.852512	3.541759	C	-2.001105	0.091053	0.530706
C	4.747357	2.975059	1.589775	H	-8.160370	2.587529	1.187087	H	-3.683382	-1.091097	-3.591409
C	5.270157	4.243009	1.355356	C	-7.287088	0.714347	0.592589	C	-1.441968	-0.668554	-2.086297
C	5.627046	4.596616	0.050703	C	-7.189061	-0.663192	0.852727	C	-0.679862	-0.049193	0.128013
Ni	4.073137	0.120689	0.951695	H	-7.799035	-2.302633	2.125410	H	-2.241608	0.387572	1.542540
H	0.993641	-0.861393	-2.669962	C	-6.483157	1.038022	-0.664763	H	-1.233247	-0.970233	-3.109112
H	3.282827	-0.579868	-2.884636	N	-6.332309	-1.269989	-0.091930	C	-0.392761	-0.431591	-1.192931
H	3.600046	-1.838457	-1.665913	C	-5.660391	2.331099	-0.576325	H	0.127585	0.137257	0.816782
H	3.604230	1.637818	-2.180952	C	-7.467479	1.091997	-1.860961	H	4.250682	-0.271477	3.415777
H	5.323101	1.450965	-2.574711	C	-5.561680	-0.249073	-0.770024	O	4.265968	0.452849	2.739375
C	-5.772776	-2.609958	0.115900								