Supplementary Material

A novel fluorescent probe based on biphenyl and rhodamine for multi-metal ions recognition and its application

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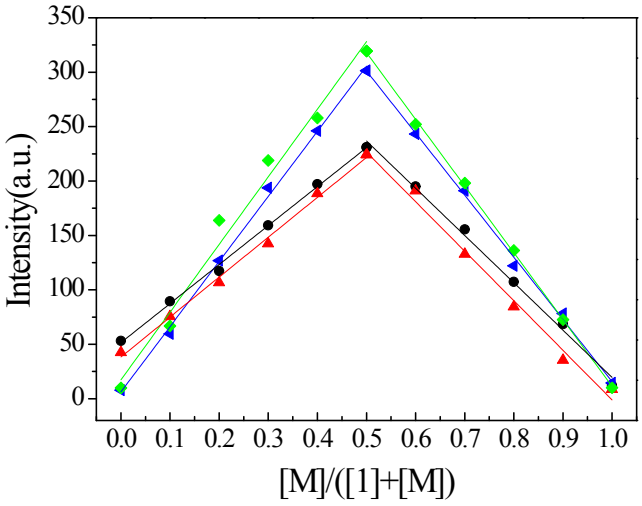


Fig.S1 The Job's plot of the probe 1 with the target metal ions.

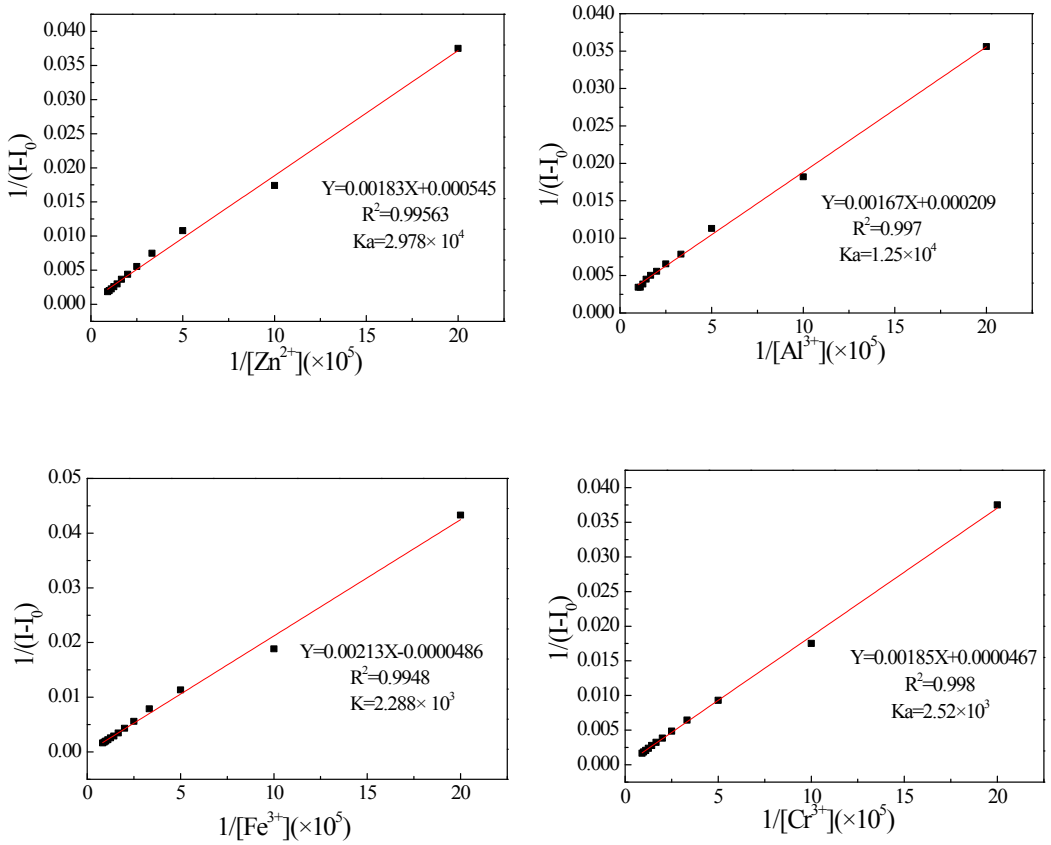


Fig S2 The linear relation of the between 1/[M] and 1/[I-I_0] for probe 1.

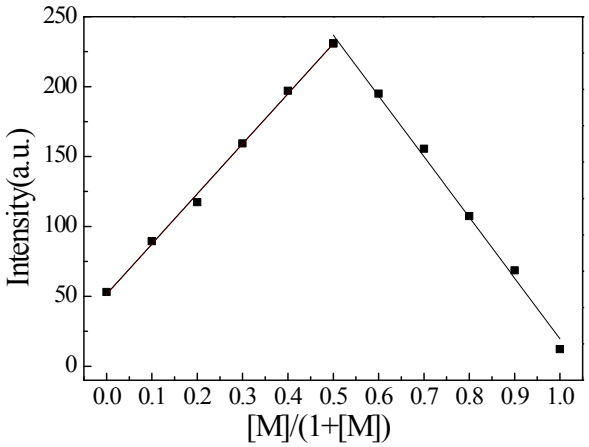


Fig.S3 The Job's plot of the probe 2 with Fe^{3+} ion.

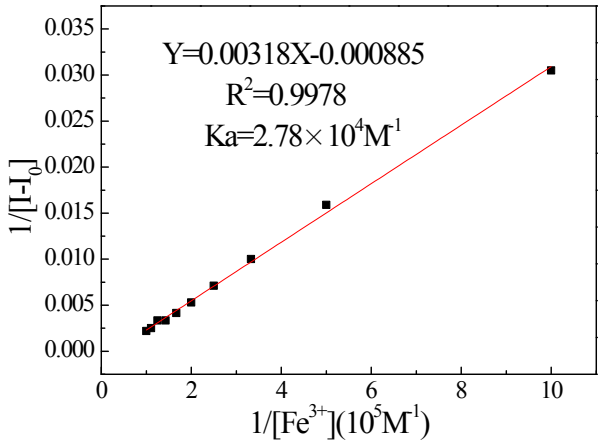


Fig. S4 The linear relation of the between $1/[Fe^{3+}]$ and $1/[I-I_0]$ for probe 2.

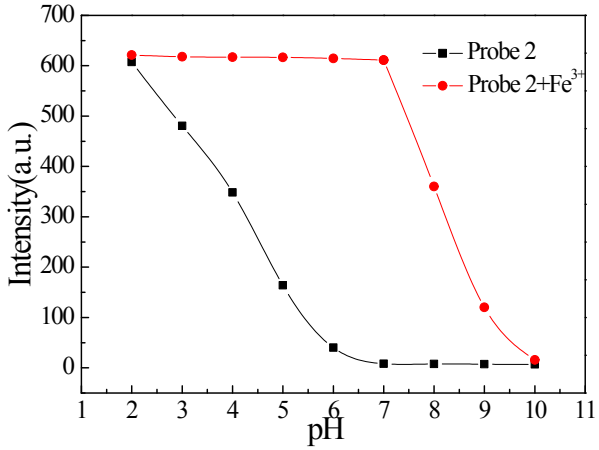


Fig.S5 The effect of system pH on the fluorescence intensity of single probe 2 and the detection of Fe^{3+} ions.

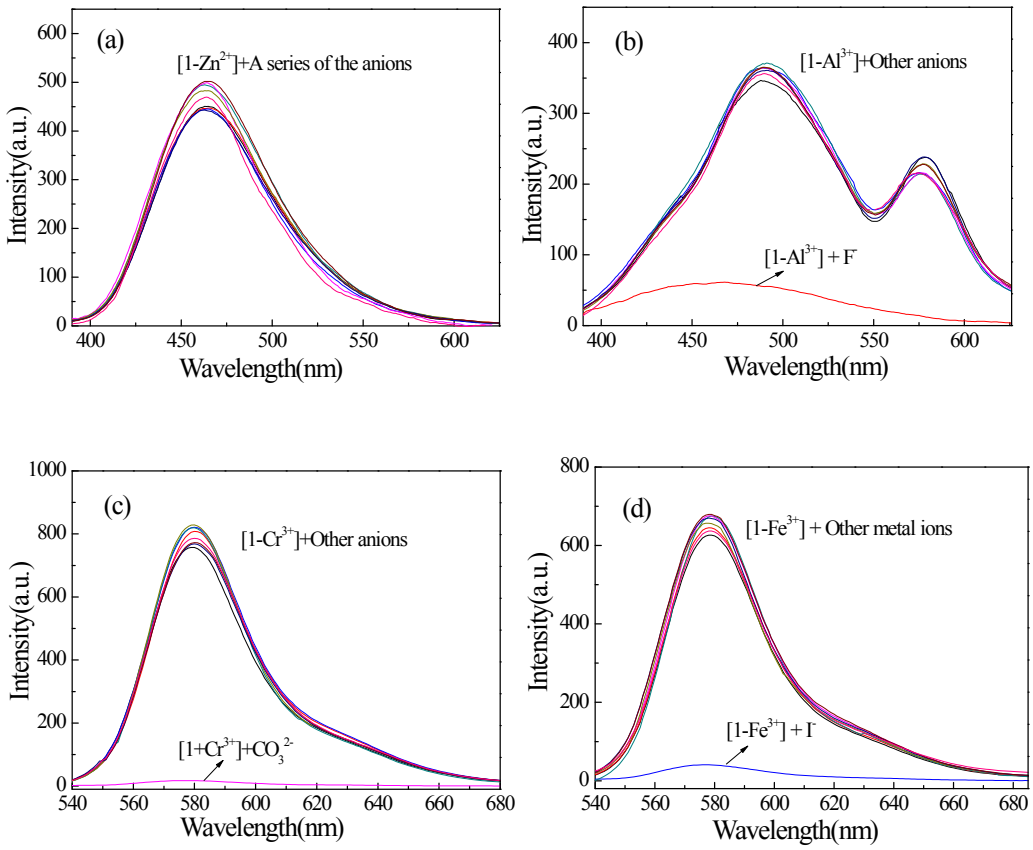


Fig. S6 The fluorescence spectra of [1-Metal] complexes before and after the addition of a series of common anions.

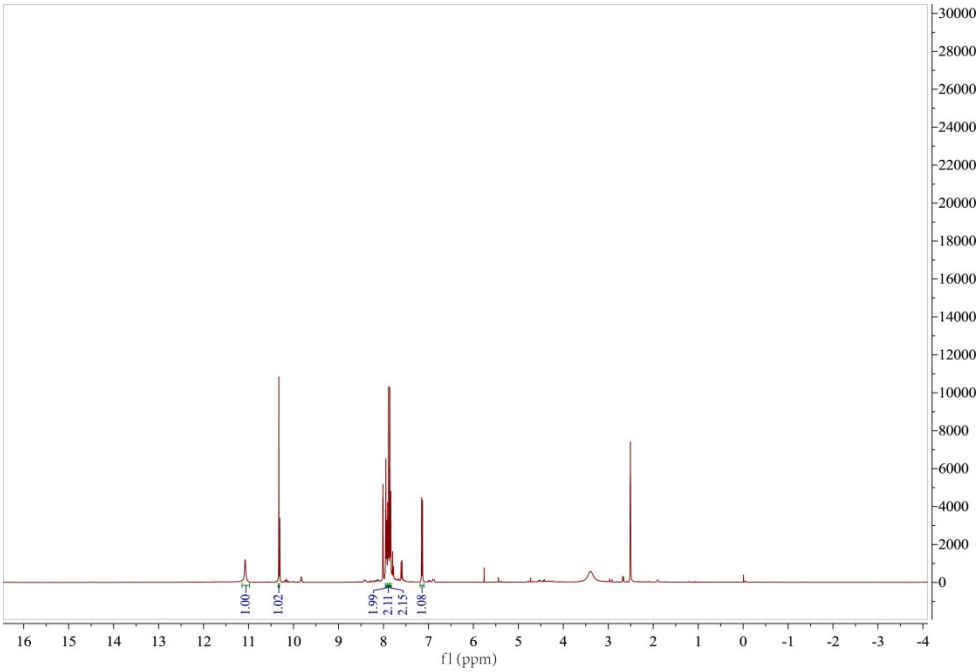


Fig. S7 The ^{1}H NMR spectrum of compound **a**

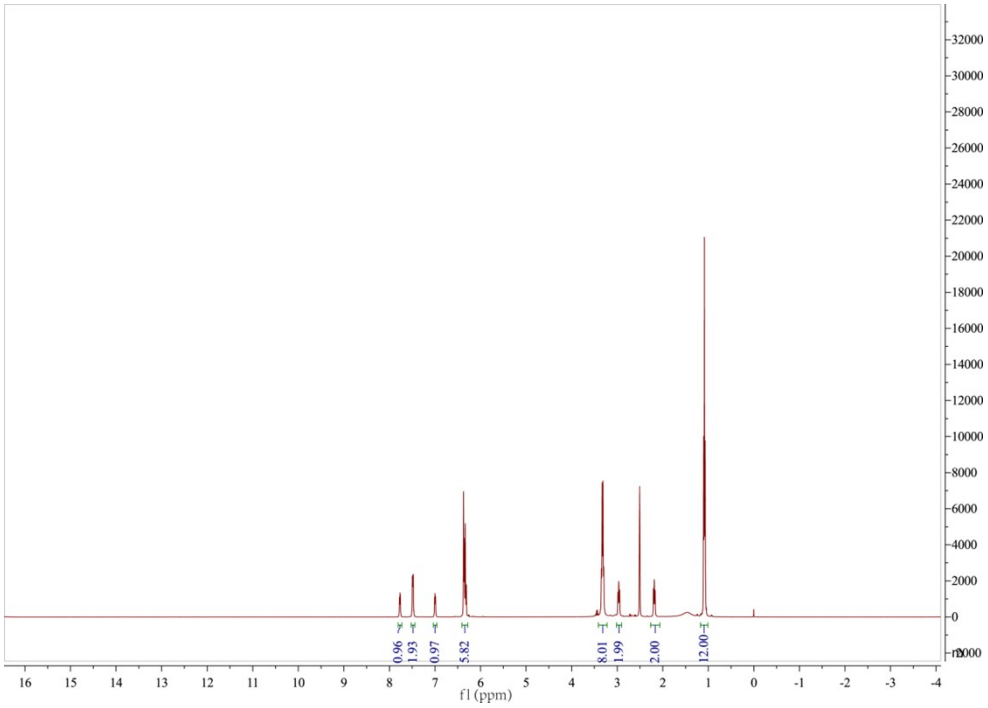


Fig S8 The ^{1}H NMR spectrum of the compound **b**

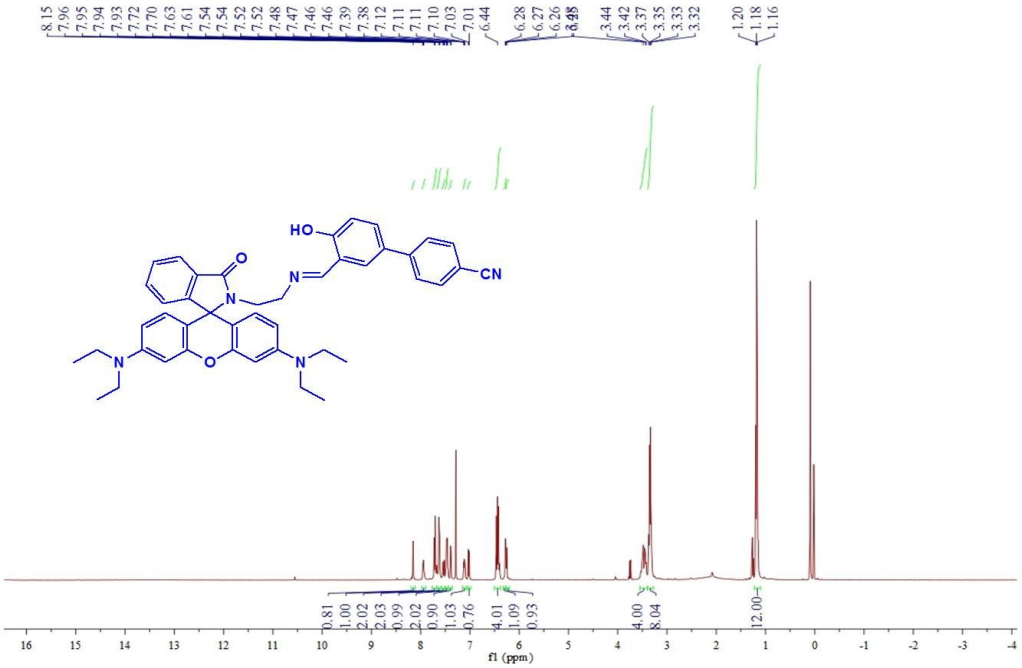


Fig.S9 The ^{1}H NMR spectrum of probe 1.

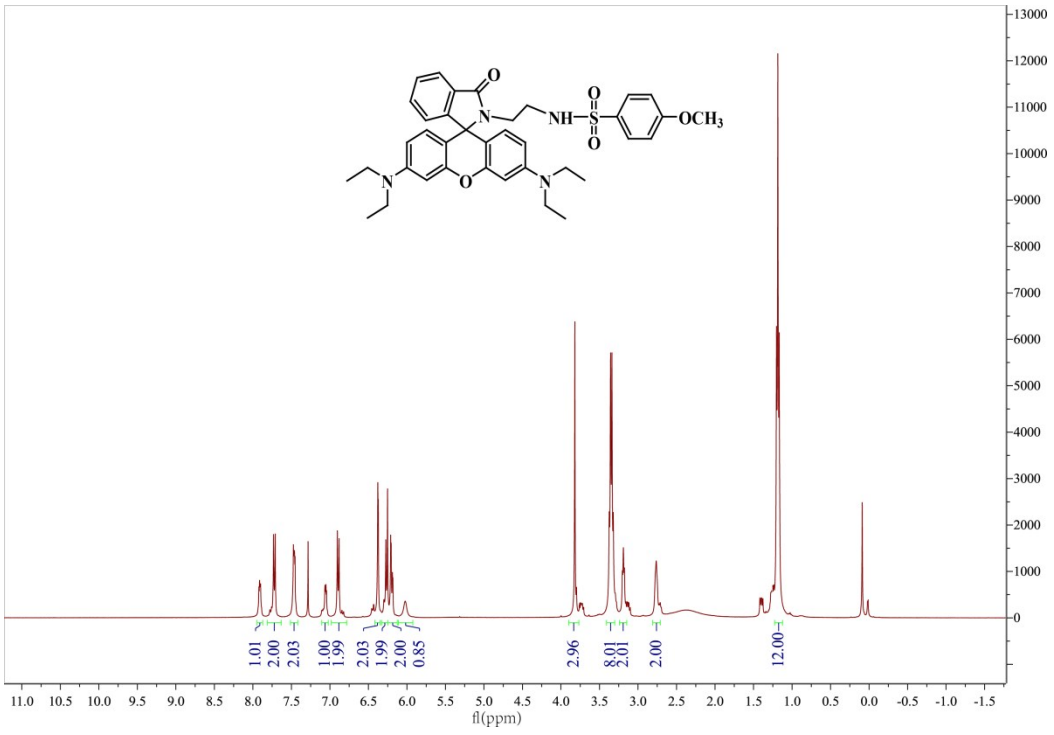


Fig S10 The ^{1}H NMR spectrum of probe 2

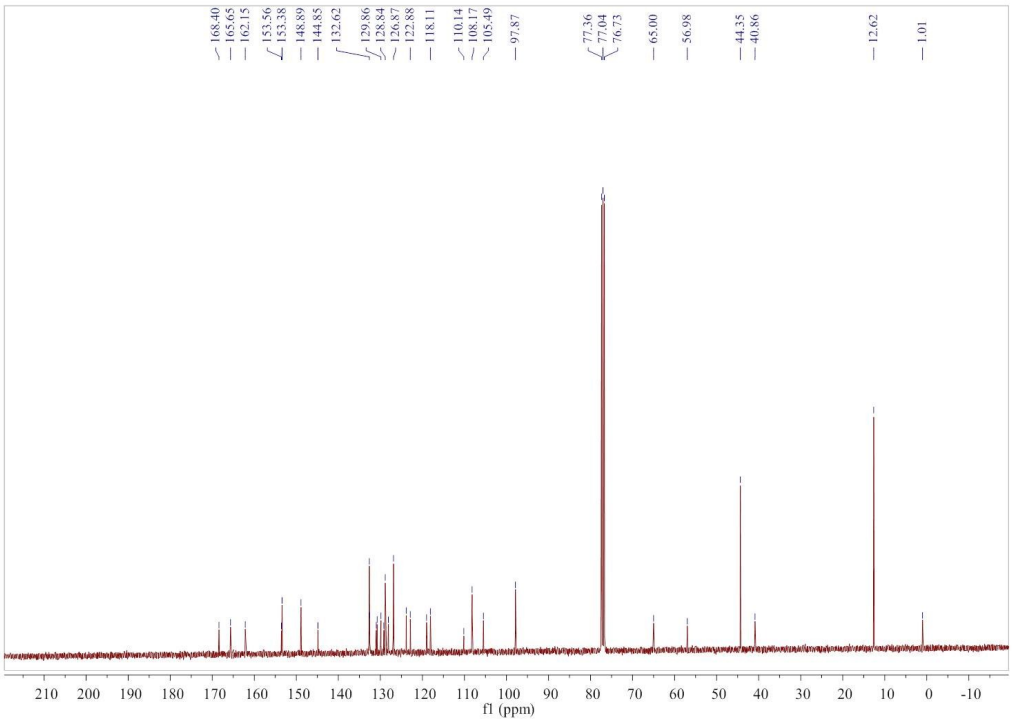


Fig.S11 The ^{13}C NMR spectrum of probe 1.

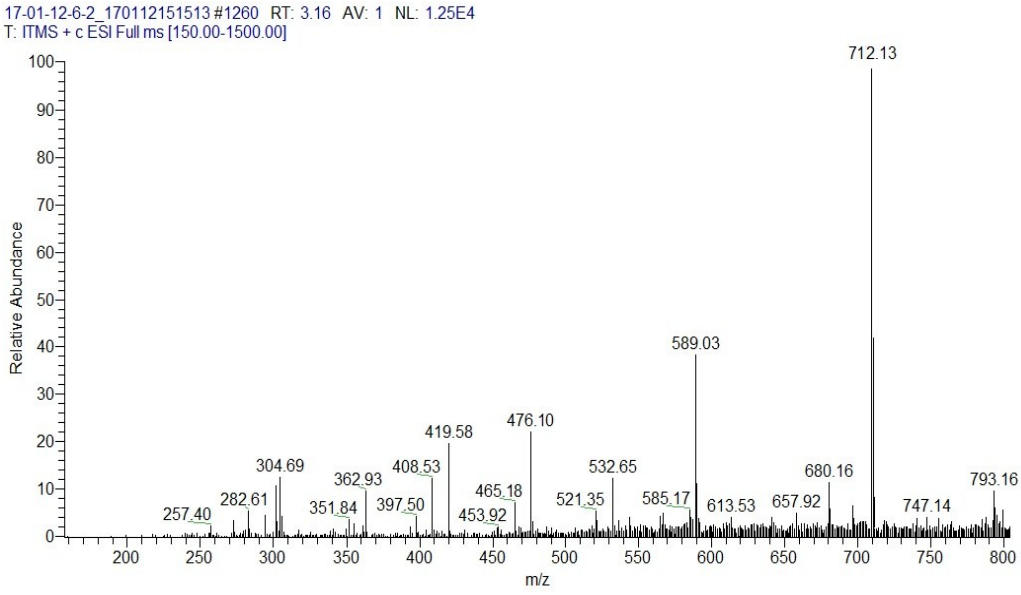
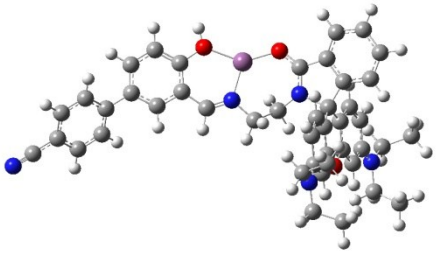
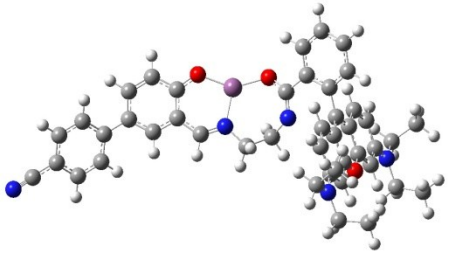


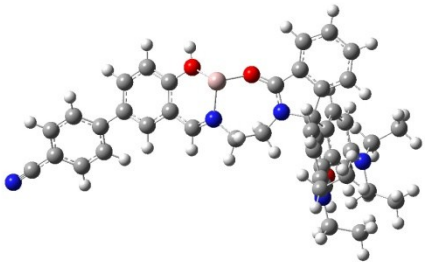
Fig. S12 The MS spectrum of probe 1



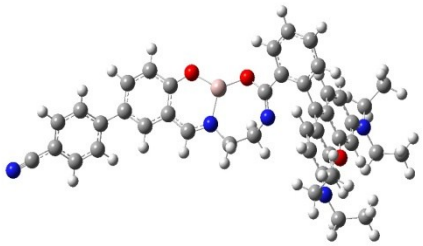
$S_1[1\text{-}Zn^{2+}]$



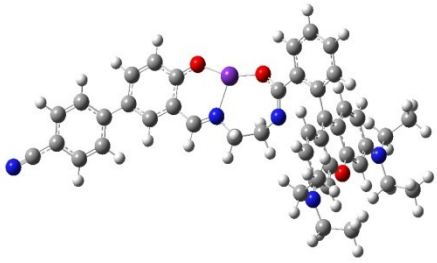
$S_2[1\text{-}Zn^{2+}]$



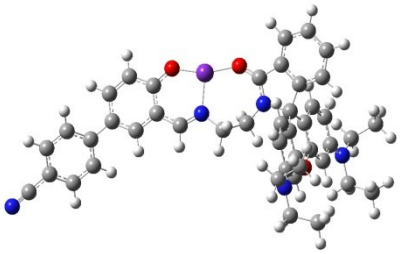
$S_1[1\text{-}Al^{3+}]$



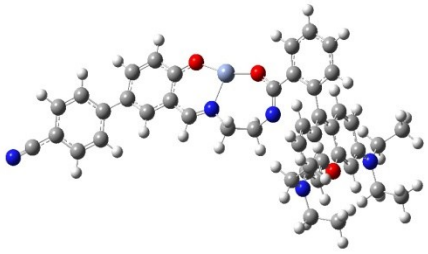
$S_2[1\text{-}Al^{3+}]$



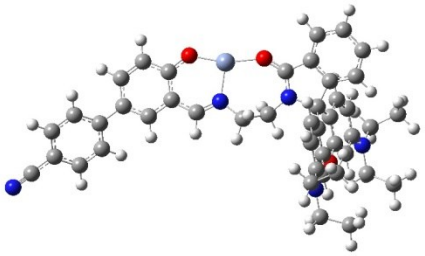
$S_1[1\text{-}Fe^{3+}]$



$S_2[1\text{-}Fe^{3+}]$



$S_1[1\text{-}Cr^{3+}]$



$S_2[1\text{-}Cr^{3+}]$

Fig. S13 The geometry optimizations for several possible complexes structures of probe 1 and metal ions with a 1:1 stoichiometry at the B3LYP/6-31G*/LANL2DZ level of theory

Table S1. XYZ Coordinates for Calculated Optimized Geometry of Probe 1 at DFT/B3LYP/6-31G*

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1C	-10.0447	-1.97543	0.23813
2C	-8.67237	-1.91647	0.54598
3C	-8.05650	-0.70341	0.85768
4C	-8.74773	0.50950	0.86677
5C	-10.11073	0.44415	0.54239
6C	-10.75202	-0.74303	0.23266
7C	-6.60401	1.59790	1.53362
8C	-6.01958	0.33090	1.48759
9C	-4.67081	0.11532	1.77652
10H	-4.31517	-0.90349	1.70155
11C	-3.82770	1.18018	2.14542
12C	-4.41207	2.47488	2.18077
13C	-5.75279	2.65586	1.88468
14H	-8.04462	-2.79729	0.55749
15H	-10.68815	1.36475	0.53335
16H	-11.80515	-0.71007	-0.01426
17H	-3.81971	3.34439	2.43462

18H	-6.16349	3.66128	1.92461
19O	-6.71592	-0.80261	1.14495
20N	-2.49507	0.97268	2.47605
21N	-10.68047	-3.18051	-0.02714
22C	-1.90183	-0.35874	2.38694
23H	-1.01859	-0.36457	3.03477
24H	-2.59709	-1.08729	2.82136
25C	-1.49824	-0.80110	0.97232
26H	-0.72224	-0.14749	0.56049
27H	-1.10390	-1.82426	0.99351
28H	-2.35356	-0.77943	0.28993
29C	-1.62031	2.09357	2.81098
30H	-2.15039	2.76982	3.49212
31H	-0.78159	1.68766	3.38674
32C	-1.07783	2.88176	1.60932
33H	-0.45529	2.24782	0.96932
34H	-1.89169	3.28150	0.99641
35H	-0.46426	3.72304	1.95366
36C	-9.93210	-4.43430	-0.03972
37H	-10.64943	-5.24291	0.13721
38H	-9.24788	-4.44777	0.81721
39C	-9.15483	-4.71725	-1.33403
40H	-8.59307	-5.65464	-1.24156
41H	-9.83296	-4.81143	-2.18860
42H	-8.44473	-3.91430	-1.55492

43C	-12.09383	-3.21913	-0.39602
44H	-12.45401	-4.23206	-0.18767
45H	-12.65713	-2.55802	0.27338
46C	-12.39649	-2.86232	-1.85916
47H	-12.02044	-1.86570	-2.11020
48H	-11.93348	-3.57916	-2.54537
49H	-13.47882	-2.87377	-2.03567
50C	-8.83938	5.01097	-1.57891
51C	-8.10153	3.91534	-2.05136
52C	-7.80027	2.83274	-1.21947
53C	-8.25303	2.86909	0.09561
54C	-8.98338	3.95928	0.56038
55C	-9.29020	5.04275	-0.25871
56H	-9.05918	5.83827	-2.24828
57H	-7.75860	3.90762	-3.08277
58H	-7.22889	1.98727	-1.59286
59H	-9.86386	5.87746	0.13358
60C	-8.07385	1.83232	1.20969
61C	-9.33823	3.73352	1.98761
62O	-9.99249	4.45563	2.73117
63N	-8.78109	2.52054	2.32941
64C	-8.99781	1.92544	3.63768
65H	-10.05501	2.02797	3.90369
66H	-8.76850	0.85817	3.56990
67C	-8.15302	2.58250	4.74627

68H	-8.40715	3.64910	4.76437
69H	-7.07977	2.48247	4.51807
70N	-8.51538	2.00910	6.02878
71C	-7.58929	1.50771	6.74829
72H	-6.53879	1.50245	6.42926
73C	-7.87237	0.90678	8.06551
74C	-8.19616	1.71519	9.17284
75C	-7.82169	-0.48051	8.24678
76C	-8.45707	1.12932	10.41634
77C	-8.07800	-1.08659	9.48206
78H	-7.54772	-1.07524	7.38146
79C	-8.39826	-0.25065	10.56793
80H	-8.71937	1.75972	11.26430
81H	-8.63275	-0.68500	11.53540
82O	-8.24626	3.06795	8.98779
83H	-8.47445	3.49338	9.82884
84C	-8.01632	-2.55916	9.64142
85C	-8.41769	-3.41783	8.60142
86C	-7.55537	-3.14094	10.83676
87C	-8.36239	-4.79858	8.74448
88H	-8.79842	-2.99575	7.67668
89C	-7.49998	-4.52009	10.99444
90H	-7.21024	-2.50265	11.64453
91C	-7.90402	-5.36396	9.94642
92H	-8.68169	-5.44637	7.93433

93H	-7.13492	-4.95248	11.92064
94C	-7.84838	-6.78702	10.10336
95N	-7.80316	-7.94262	10.23371

Table S2. XYZ Coordinates for Calculated Optimized Geometry of S_0[1-Zn^{2+}]at DFT/B3LYP/ LANL2DZ

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1C	-10.064167	-1.925514	-1.032841
2C	-8.711684	-2.011067	-0.622727
3C	-8.151526	-1.045997	0.205747
4C	-8.876260	0.062031	0.674359
5C	-10.219639	0.149840	0.252059
6C	-10.803906	-0.793280	-0.566546
7C	-6.758405	0.880602	1.691562
8C	-6.139042	-0.270584	1.182505
9C	-4.770781	-0.496383	1.293936
10H	-4.389140	-1.398610	0.836614
11C	-3.923654	0.436085	1.937660
12C	-4.548739	1.615166	2.451710
13C	-5.909700	1.812948	2.322901
14H	-8.061822	-2.811029	-0.949101
15H	-10.818923	0.999657	0.567739
16H	-11.832438	-0.647692	-0.867019

17H	-3.958007	2.389598	2.922372
18H	-6.334548	2.738993	2.703250
19O	-6.832878	-1.251831	0.524069
20N	-2.577182	0.217171	2.070836
21N	-10.637779	-2.880322	-1.827968
22C	-1.945831	-0.985589	1.506873
23H	-1.018791	-1.148852	2.063659
24H	-2.583033	-1.849721	1.724734
25C	-1.638522	-0.911384	0.005488
26H	-0.920701	-0.115450	-0.213525
27H	-1.201765	-1.858703	-0.328820
28H	-2.540718	-0.725043	-0.585704
29C	-1.694456	1.231595	2.665795
30H	-2.164153	1.619726	3.576863
31H	-0.790712	0.711019	2.994307
32C	-1.311996	2.385061	1.729047
33H	-0.754304	2.021776	0.861136
34H	-2.194249	2.919962	1.363015
35H	-0.676205	3.100123	2.262486
36C	-9.846934	-4.003146	-2.355277
37H	-10.554435	-4.792358	-2.621995
38H	-9.231246	-4.410945	-1.545711
39C	-8.977070	-3.657897	-3.571568
40H	-8.406810	-4.541110	-3.878981
41H	-9.590897	-3.341070	-4.419763

42H	-8.267824	-2.854710	-3.348573
43C	-12.040193	-2.774542	-2.261532
44H	-12.376215	-3.788390	-2.494861
45H	-12.647800	-2.445039	-1.412289
46C	-12.270060	-1.862489	-3.473708
47H	-11.929125	-0.839974	-3.281936
48H	-11.742031	-2.234595	-4.356602
49H	-13.338852	-1.827138	-3.710953
50C	-9.603711	5.134581	1.025110
51C	-8.856185	4.568510	-0.021238
52C	-8.360784	3.261457	0.054057
53C	-8.631610	2.524848	1.200127
54C	-9.373768	3.096131	2.241329
55C	-9.870986	4.401993	2.178930
56H	-9.974307	6.150159	0.930676
57H	-8.659387	5.159513	-0.910757
58H	-7.786094	2.836755	-0.762841
59H	-10.448927	4.821928	2.995858
60C	-8.248038	1.091047	1.578386
61C	-9.483283	2.115878	3.308997
62O	-10.098395	2.333901	4.424898
63N	-8.841575	0.993141	2.908698
64C	-8.872941	-0.281732	3.667135
65H	-9.887004	-0.493334	4.036609
66H	-8.673293	-1.042976	2.907176

67C	-7.838507	-0.428100	4.801437
68H	-6.983188	0.225176	4.615948
69H	-7.479316	-1.461791	4.851574
70C	-7.495173	0.032934	7.216902
71C	-6.507821	-0.367307	6.995698
72H	-7.750807	0.530274	8.472738
73C	-8.989520	1.241445	8.862977
74C	-6.714646	0.360825	9.472009
75C	-9.131528	1.619316	10.216373
76C	-6.878566	0.750804	10.776188
77H	-5.786621	-0.107026	9.157251
78C	-8.127375	1.381243	11.126661
79H	-10.052293	2.113343	10.507812
80H	-8.284362	1.674599	12.160379
81O	-9.925844	1.556165	8.018386
82C	-5.842377	0.532342	11.810304
83C	-5.042873	-0.625008	11.792834
84C	-5.632715	1.483721	12.825526
85C	-4.056577	-0.824209	12.750584
86H	-5.217376	-1.395156	11.047217
87C	-4.644095	1.296066	13.784456
88H	-6.219994	2.397001	12.853037
89C	-3.847752	0.139055	13.752905
90H	-3.453430	-1.725742	12.739131
91H	-4.479963	2.040745	14.555869

92C	-2.828289	-0.062283	14.739769
93N	-1.997004	-0.226552	15.535757
94Zn	-9.753380	1.633025	6.133099
95N	-8.431730	-0.056450	6.133186
96H	-9.128249	-0.770764	6.381014

Table S2. XYZ Coordinates for Calculated Optimized Geometry of S_0[1-Al^{3+}]at DFT/B3LYP/ LANL2DZ

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1C	-9.94154	-1.63435	-1.27275
2C	-8.53963	-1.76545	-1.05535
3C	-7.82059	-0.72431	-0.50897
4C	-8.41701	0.49214	-0.13053
5C	-9.80338	0.62582	-0.36357
6C	-10.55102	-0.38290	-0.91278
7C	-6.15540	1.39661	0.17472
8C	-5.66127	0.14472	-0.23262
9C	-4.33152	-0.07042	-0.52571
10H	-4.04959	-1.05923	-0.86158
11C	-3.39191	0.99560	-0.42957
12C	-3.89548	2.28258	-0.03365
13C	-5.22512	2.45599	0.25142
14H	-7.98962	-2.64848	-1.35253

15H	-10.29622	1.55662	-0.09848
16H	-11.61146	-0.22814	-1.06003
17H	-3.23096	3.13283	0.03877
18H	-5.57393	3.44297	0.54131
19O	-6.47942	-0.94209	-0.36521
20N	-2.08709	0.80711	-0.69860
21N	-10.66926	-2.63722	-1.79537
22C	-1.57579	-0.50776	-1.11176
23H	-0.51326	-0.52680	-0.86411
24H	-2.05377	-1.27438	-0.49671
25C	-1.77689	-0.78562	-2.60323
26H	-1.20533	-0.08494	-3.21514
27H	-1.42481	-1.79479	-2.83099
28H	-2.83069	-0.71200	-2.88673
29C	-1.13501	1.92949	-0.70849
30H	-1.29168	2.52871	0.19278
31H	-0.13774	1.49576	-0.62437
32C	-1.23213	2.78865	-1.97100
33H	-0.98541	2.20843	-2.86225
34H	-2.23403	3.20740	-2.09892
35H	-0.51938	3.61371	-1.89752
36C	-10.07560	-3.94917	-2.08537
37H	-10.87143	-4.68812	-1.97111
38H	-9.33119	-4.17061	-1.31830
39C	-9.47435	-4.02764	-3.49012

40H	-9.01088	-5.00734	-3.62917
41H	-10.24409	-3.90999	-4.25598
42H	-8.71393	-3.25586	-3.64051
43C	-12.06712	-2.43498	-2.21281
44H	-12.48708	-3.42615	-2.38814
45H	-12.62538	-2.00170	-1.37709
46C	-12.19796	-1.57867	-3.47435
47H	-11.76311	-0.58500	-3.33836
48H	-11.70596	-2.05514	-4.32457
49H	-13.25693	-1.46082	-3.71673
50C	-9.24648	5.23759	1.28248
51C	-8.79561	4.63523	0.09931
52C	-8.24852	3.34946	0.09076
53C	-8.16379	2.68228	1.30233
54C	-8.61074	3.28751	2.47492
55C	-9.15946	4.56803	2.49823
56H	-9.66701	6.23658	1.24482
57H	-8.87525	5.18302	-0.83427
58H	-7.90432	2.89356	-0.83270
59H	-9.50572	5.01872	3.42247
60C	-7.60592	1.57685	0.52875
61C	-8.38753	2.35120	3.56064
62O	-8.70693	2.60785	4.78335
63N	-7.82737	1.23944	3.11699
64C	-7.51511	0.01291	3.85764

65H	-8.44631	-0.52198	4.08030
66H	-6.94476	-0.60925	3.16366
67C	-6.69208	0.20481	5.14243
68H	-6.09535	1.12283	5.07611
69H	-5.98739	-0.62420	5.25192
70C	-6.99360	1.22951	7.45087
71H	-5.90834	1.22225	7.50395
72C	-7.70295	0.98128	8.74458
73C	-9.09784	1.34373	8.79629
74C	-7.09003	0.55472	9.90412
75C	-9.83525	1.19920	9.98945
76C	-7.80360	0.45194	11.12988
77H	-6.02577	0.34328	9.88406
78C	-9.19560	0.77439	11.12550
79H	-10.89053	1.44849	9.98360
80H	-9.77573	0.65253	12.03299
81O	-9.67263	1.84595	7.71317
82C	-7.14758	0.03117	12.34907
83C	-5.94296	-0.72289	12.31493
84C	-7.69026	0.37260	13.61866
85C	-5.32106	-1.12005	13.47638
86H	-5.52528	-1.03974	11.36619
87C	-7.06222	-0.00368	14.78477
88H	-8.58372	0.98251	13.68384
89C	-5.87400	-0.75793	14.72200

90H	-4.41538	-1.71552	13.44921
91H	-7.46629	0.27994	15.75041
92C	-5.22148	-1.16175	15.92683
93N	-4.68721	-1.49213	16.90053
94Al	-8.45655	2.03213	6.43221
95N	-7.54813	0.29514	6.34268
96H	-7.82008	-0.62769	6.68640

Table S2. XYZ Coordinates for Calculated Optimized Geometry of S_0[1-Fe^{3+}]at DFT/B3LYP/ LANL2DZ

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1C	-9.74814	-1.92793	-1.51154
2C	-8.39419	-1.94925	-1.08510
3C	-7.82764	-0.82567	-0.50875
4C	-8.56896	0.35538	-0.31201
5C	-9.91468	0.36777	-0.72904
6C	-10.50345	-0.72657	-1.31416
7C	-6.42690	1.45497	0.23360
8C	-5.79714	0.22220	0.04009
9C	-4.42596	0.06667	0.01074
10H	-4.04005	-0.92400	-0.18966
11C	-3.57296	1.18735	0.18207
12C	-4.21015	2.45671	0.36723

13C	-5.57910	2.56887	0.38987
14H	-7.74799	-2.80270	-1.24761
15H	-10.50199	1.27022	-0.58744
16H	-11.54578	-0.67851	-1.60101
17H	-3.61620	3.35467	0.46896
18H	-6.02069	3.55497	0.51382
19O	-6.52804	-0.93491	-0.15250
20N	-2.22788	1.06527	0.17604
21N	-10.31391	-3.01176	-2.09640
22C	-1.59192	-0.23801	-0.03981
23H	-0.58686	-0.17657	0.38271
24H	-2.12512	-0.98817	0.55257
25C	-1.51972	-0.64433	-1.51078
26H	-0.87796	0.03795	-2.07303
27H	-1.09975	-1.64938	-1.60147
28H	-2.50963	-0.63888	-1.97724
29C	-1.35794	2.24832	0.21551
30H	-1.68465	2.90043	1.03226
31H	-0.36153	1.89697	0.48993
32C	-1.29436	3.00986	-1.10753
33H	-0.85736	2.39064	-1.89402
34H	-2.28603	3.32916	-1.44084
35H	-0.66922	3.89930	-0.99350
36C	-9.62881	-4.31187	-2.16490
37H	-10.40476	-5.07054	-2.03503

38H	-8.95127	-4.39610	-1.31587
39C	-8.90671	-4.50498	-3.50038
40H	-8.39966	-5.47267	-3.48882
41H	-9.61084	-4.50717	-4.33577
42H	-8.16262	-3.72112	-3.66722
43C	-11.60311	-2.92438	-2.81061
44H	-11.88733	-3.94935	-3.05167
45H	-12.35776	-2.53466	-2.12105
46C	-11.51089	-2.08404	-4.08716
47H	-11.26642	-1.04069	-3.87378
48H	-10.75799	-2.48397	-4.76978
49H	-12.47910	-2.11406	-4.59311
50C	-9.80519	5.16565	0.47980
51C	-9.19501	4.45573	-0.56375
52C	-8.61119	3.20309	-0.35666
53C	-8.65629	2.67782	0.92451
54C	-9.25998	3.39155	1.96059
55C	-9.84251	4.64271	1.76766
56H	-10.24705	6.13549	0.27885
57H	-9.17058	4.89470	-1.55610
58H	-8.12771	2.66991	-1.16954
59H	-10.30729	5.18260	2.58590
60C	-7.92010	1.56288	0.33585
61C	-9.09970	2.60391	3.17314
62O	-9.44495	2.97146	4.35135

63N	-8.51460	1.45163	2.89694
64C	-8.11479	0.47138	3.89061
65H	-9.00286	0.08495	4.40562
66H	-7.66921	-0.36295	3.34282
67C	-7.08509	1.00418	4.90892
68H	-6.57261	1.87798	4.49020
69H	-6.32546	0.23833	5.09016
70C	-7.22027	0.84460	7.27716
71H	-6.41535	0.11518	7.15756
72C	-7.60840	1.08140	8.64905
73C	-8.56279	2.01516	9.07267
74C	-6.94069	0.33976	9.64097
75C	-8.84962	2.21371	10.40620
76C	-7.20610	0.50621	11.00050
77H	-6.17474	-0.36890	9.33567
78C	-8.17189	1.45713	11.36150
79H	-9.59919	2.93711	10.71871
80H	-8.41606	1.59845	12.41010
81C	-6.48892	-0.28629	12.02414
82C	-6.21985	-1.64233	11.80480
83C	-6.07662	0.31560	13.21879
84C	-5.54814	-2.38891	12.76175
85H	-6.56991	-2.12972	10.89891
86C	-5.39854	-0.42296	14.17840
87H	-6.25552	1.37310	13.39103

88C	-5.13371	-1.77723	13.94976
89H	-5.34999	-3.44321	12.60369
90H	-5.06619	0.04126	15.10046
91C	-4.42898	-2.54752	14.93964
92N	-3.85910	-3.16866	15.73054
93Fe	-9.12284	2.69837	6.15174
94N	-7.69151	1.38152	6.19914
95O	-9.24006	2.77207	8.09931
96H	-9.83441	3.41483	8.53325

Table S2. XYZ Coordinates for Calculated Optimized Geometry of S_0[1-Cr^{3+}]at DFT/B3LYP/ LANL2DZ

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1C	-9.64093	-2.09983	-1.54429
2C	-8.29176	-2.11856	-1.10375
3C	-7.73079	-0.99151	-0.52826
4C	-8.47335	0.19143	-0.34987
5C	-9.81397	0.20162	-0.78177
6C	-10.39767	-0.89686	-1.36452
7C	-6.33724	1.29135	0.22586
8C	-5.70750	0.05654	0.04961
9C	-4.33638	-0.10386	0.04910
10H	-3.95008	-1.09652	-0.13964

11C	-3.48405	1.01472	0.23386
12C	-4.12014	2.28632	0.40090
13C	-5.48941	2.40290	0.39503
14H	-7.64400	-2.97311	-1.25240
15H	-10.40162	1.10606	-0.65504
16H	-11.43607	-0.84885	-1.66507
17H	-3.52532	3.18296	0.51064
18H	-5.93035	3.39080	0.50673
19O	-6.43657	-1.10049	-0.15488
20N	-2.13867	0.88910	0.25678
21N	-10.20118	-3.18631	-2.13027
22C	-1.50133	-0.41586	0.05601
23H	-0.50497	-0.35627	0.49903
24H	-2.04879	-1.16363	0.63843
25C	-1.39986	-0.82664	-1.41196
26H	-0.74716	-0.14636	-1.96383
27H	-0.97840	-1.83213	-1.49067
28H	-2.38030	-0.82299	-1.89789
29C	-1.26874	2.07098	0.31069
30H	-1.61250	2.72676	1.11752
31H	-0.27868	1.72001	0.60783
32C	-1.17787	2.82904	-1.01241
33H	-0.73203	2.20574	-1.79064
34H	-2.16206	3.15448	-1.36184
35H	-0.54887	3.71453	-0.88903

36C	-9.51943	-4.48951	-2.18175
37H	-10.29650	-5.24736	-2.05447
38H	-8.85005	-4.56947	-1.32623
39C	-8.78076	-4.69387	-3.50659
40H	-8.27104	-5.65981	-3.47850
41H	-9.47328	-4.70651	-4.35142
42H	-8.03669	-3.90953	-3.67048
43C	-11.48718	-3.10008	-2.85155
44H	-11.77601	-4.12476	-3.08788
45H	-12.24289	-2.70355	-2.16686
46C	-11.39109	-2.26823	-4.13277
47H	-11.12728	-1.22799	-3.92871
48H	-10.65114	-2.68598	-4.81862
49H	-12.36361	-2.28545	-4.63056
50C	-9.83276	5.14509	0.36755
51C	-9.18204	4.43022	-0.64756
52C	-8.59117	3.18702	-0.40725
53C	-8.66950	2.67636	0.87844
54C	-9.31353	3.39492	1.88615
55C	-9.90396	4.63629	1.65971
56H	-10.27920	6.10723	0.14116
57H	-9.13097	4.85752	-1.64391
58H	-8.07846	2.64966	-1.19922
59H	-10.39986	5.17978	2.45702
60C	-7.83201	1.40487	0.29635

61C	-9.18369	2.62580	3.11499
62O	-9.56523	2.99220	4.27672
63N	-8.57013	1.47688	2.86881
64C	-8.19076	0.51108	3.88481
65H	-9.08734	0.16192	4.41230
66H	-7.77400	-0.35039	3.35653
67C	-7.14078	1.03375	4.89074
68H	-6.61794	1.89483	4.45893
69H	-6.39250	0.25571	5.07065
70C	-7.23866	0.92202	7.26671
71H	-6.42966	0.19557	7.14931
72C	-7.60720	1.17078	8.64498
73C	-8.53291	2.11852	9.11230
74C	-6.93355	0.39857	9.61096
75C	-8.77525	2.29098	10.45865
76C	-7.15950	0.53858	10.98037
77H	-6.19047	-0.31958	9.27358
78C	-8.09264	1.50289	11.38430
79H	-9.49988	3.02410	10.80558
80H	-8.30842	1.63073	12.44084
81C	-6.43377	-0.29388	11.96525
82C	-6.19994	-1.64940	11.70530
83C	-5.97630	0.26841	13.16278
84C	-5.51832	-2.43361	12.62406
85H	-6.58554	-2.10620	10.79799

86C	-5.28820	-0.50811	14.08444
87H	-6.12763	1.32473	13.36614
88C	-5.05771	-1.86117	13.81456
89H	-5.34635	-3.48728	12.43437
90H	-4.92067	-0.07468	15.00800
91C	-4.33982	-2.67090	14.76222
92N	-3.75784	-3.32534	15.51673
93Cr	-9.25177	2.77806	6.15195
94N	-7.73023	1.43400	6.18468
95O	-9.22834	2.92279	8.18914
96H	-9.74400	3.59386	8.67629