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Novel recognition mechanism based on oxidative addition of Pt(II) complex-based luminescent probes for hypochlorite ion detection

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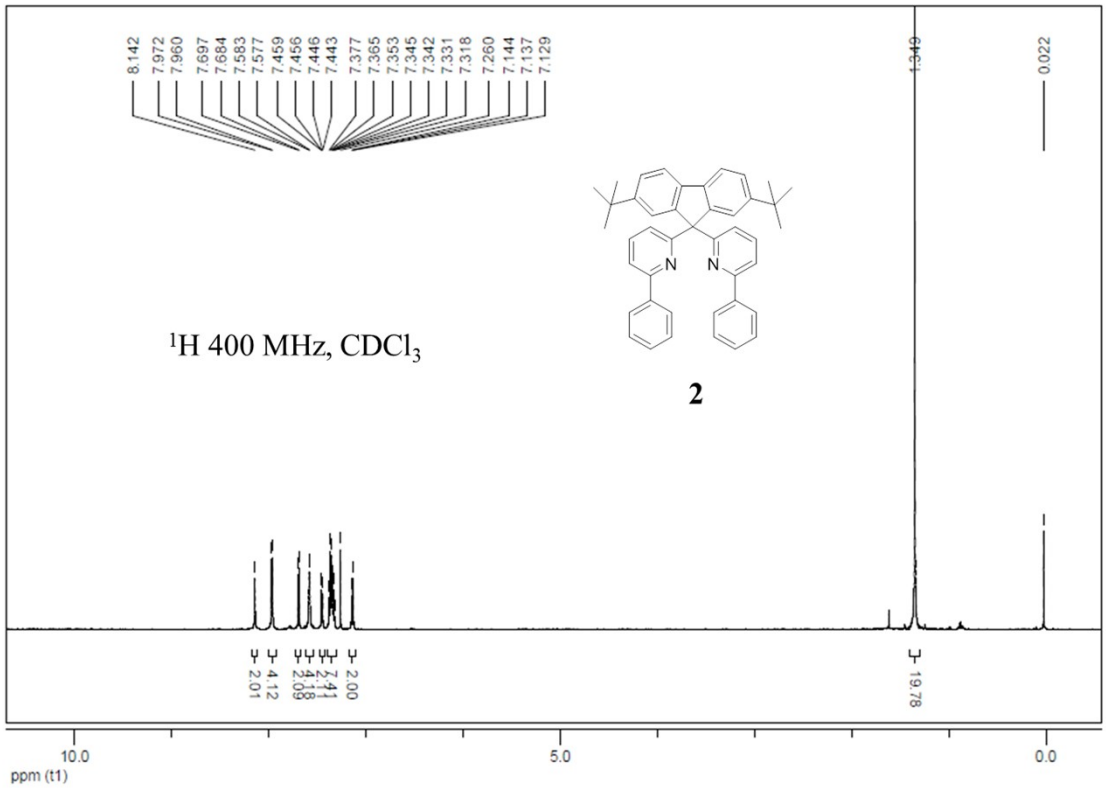
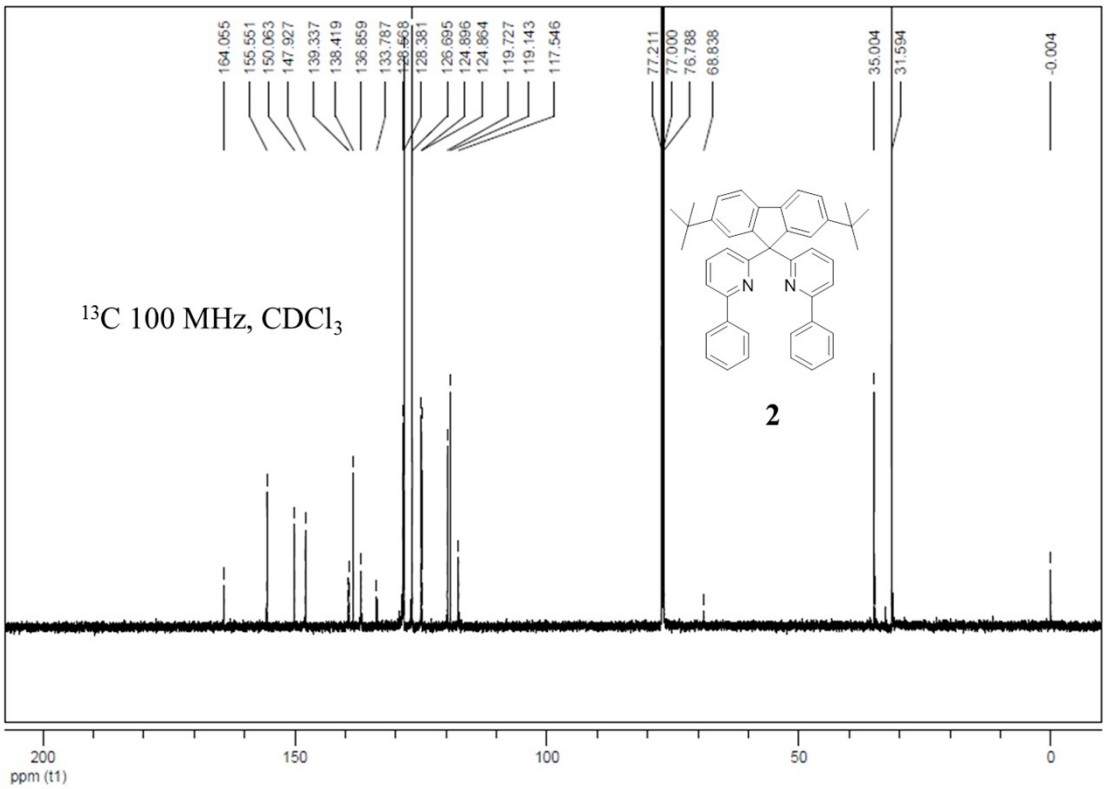
Fig. S1 ^{1}H NMR, ^{13}C NMR and ESI-MS spectra of intermediates **2.**





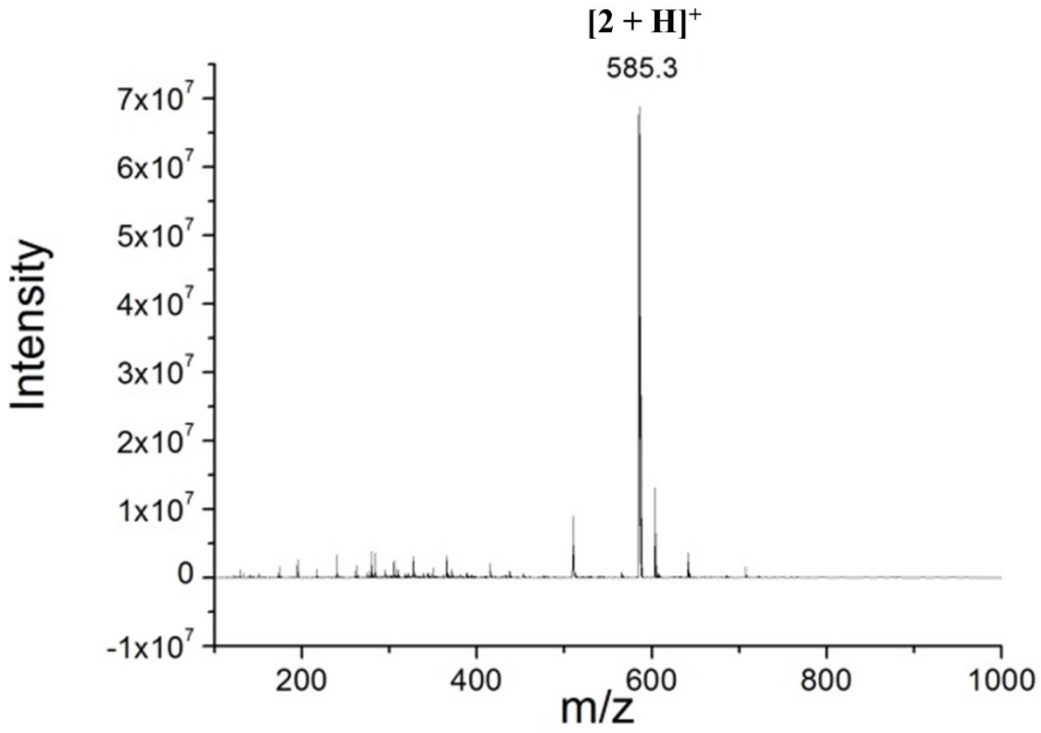
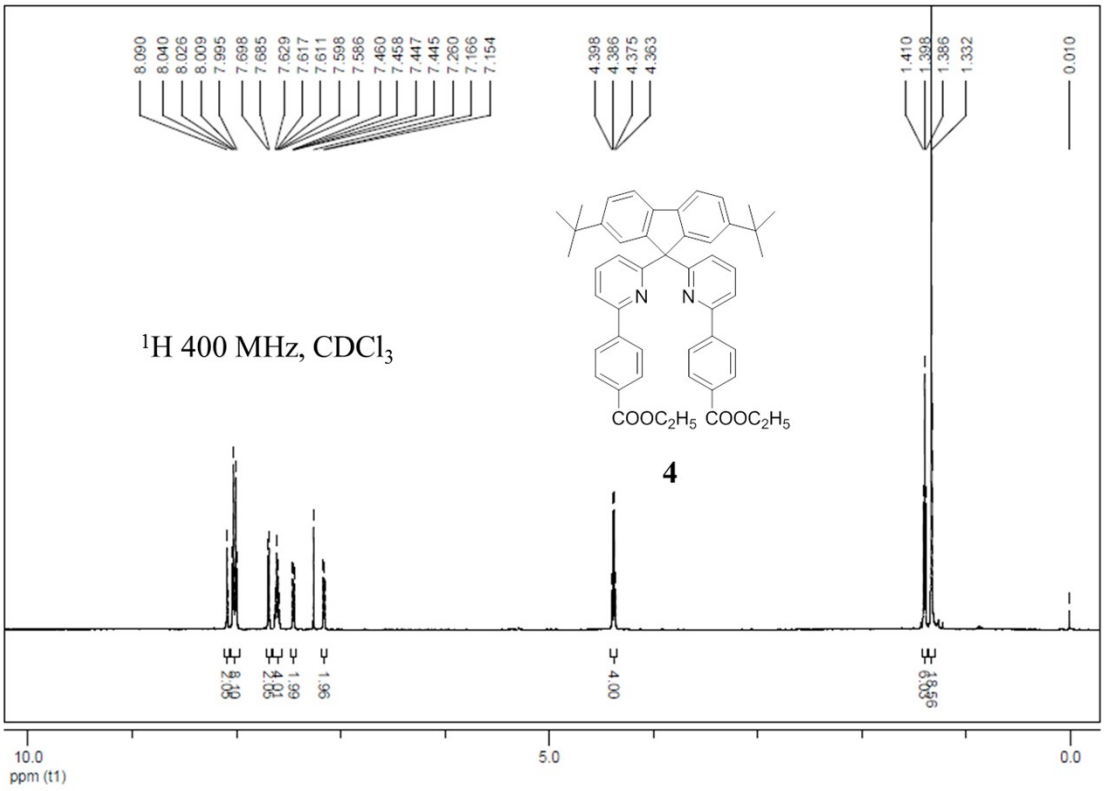
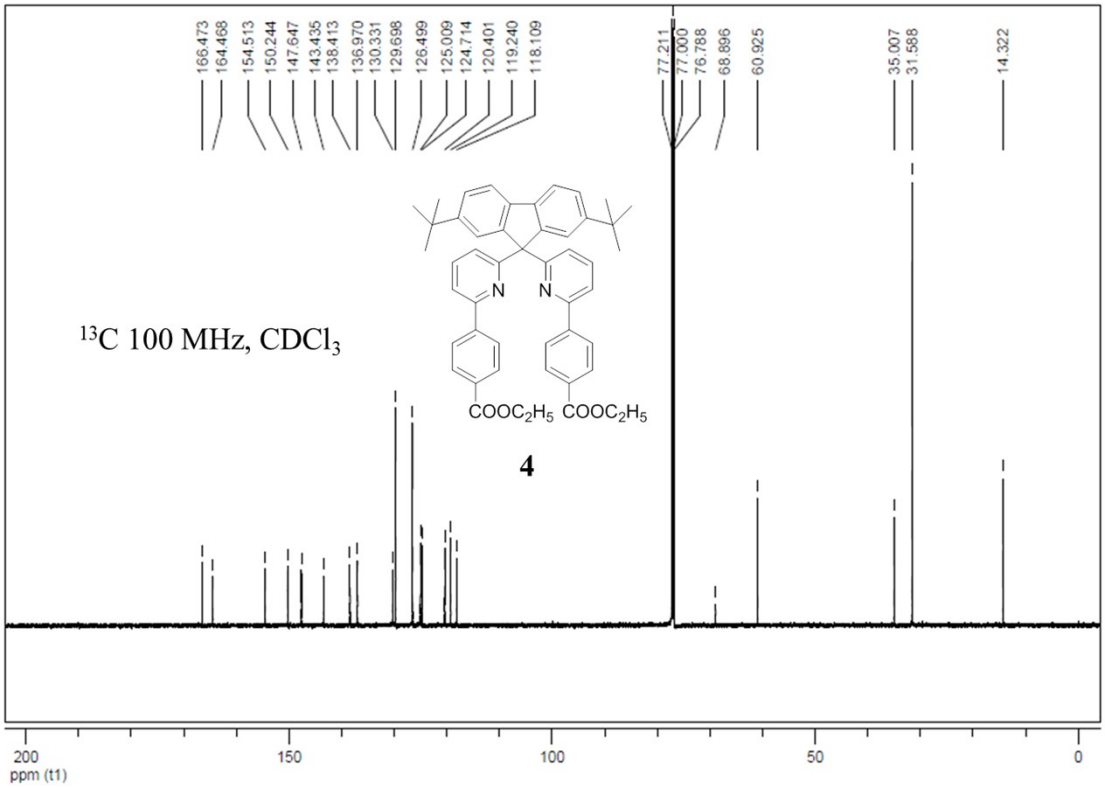


Fig. S2 ^{1}H NMR, ^{13}C NMR and ESI-MS spectra of intermediates **4.**

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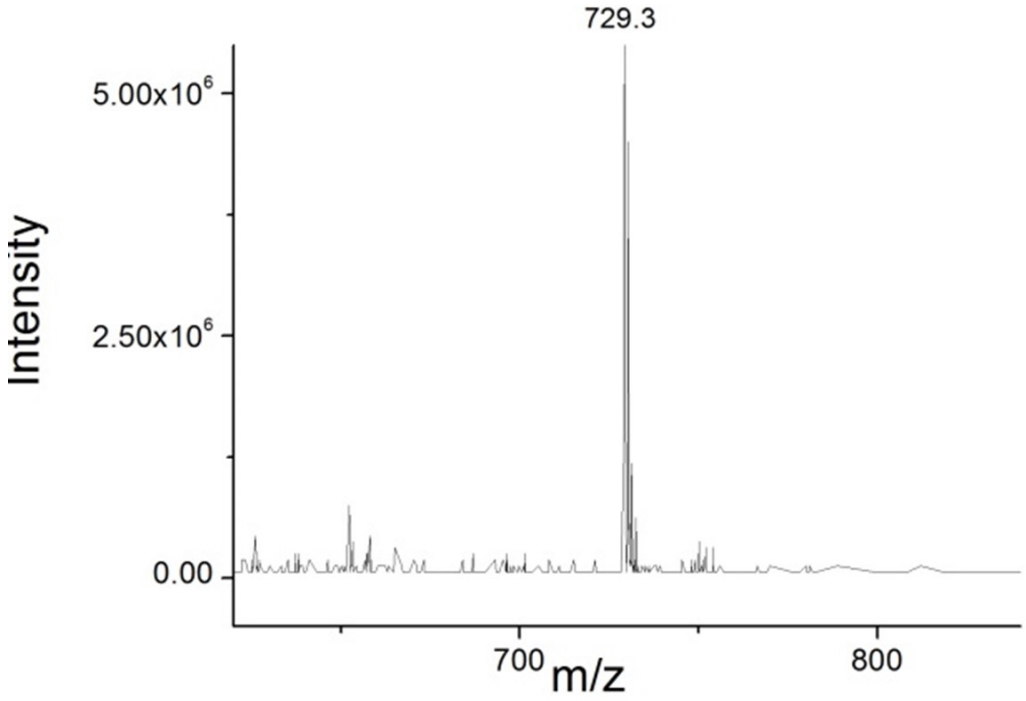
164.468
154.513
150.244
147.647
143.435
138.413
136.970
130.331
129.698
126.499
125.009
124.714
120.401
119.240
118.109
77.211
77.000
76.788
68.896
60.925
35.007
31.588
14.322
^{13}C 100 MHz, $CDCl_3$
N
N
$COOC_2H_5$ $COOC_2H_5$
200
ppm (t1)
150
100
50
0

4

$[4 + H]^+$


729.3
5.00x10^6
2.50x10^6
0.00
Intensity
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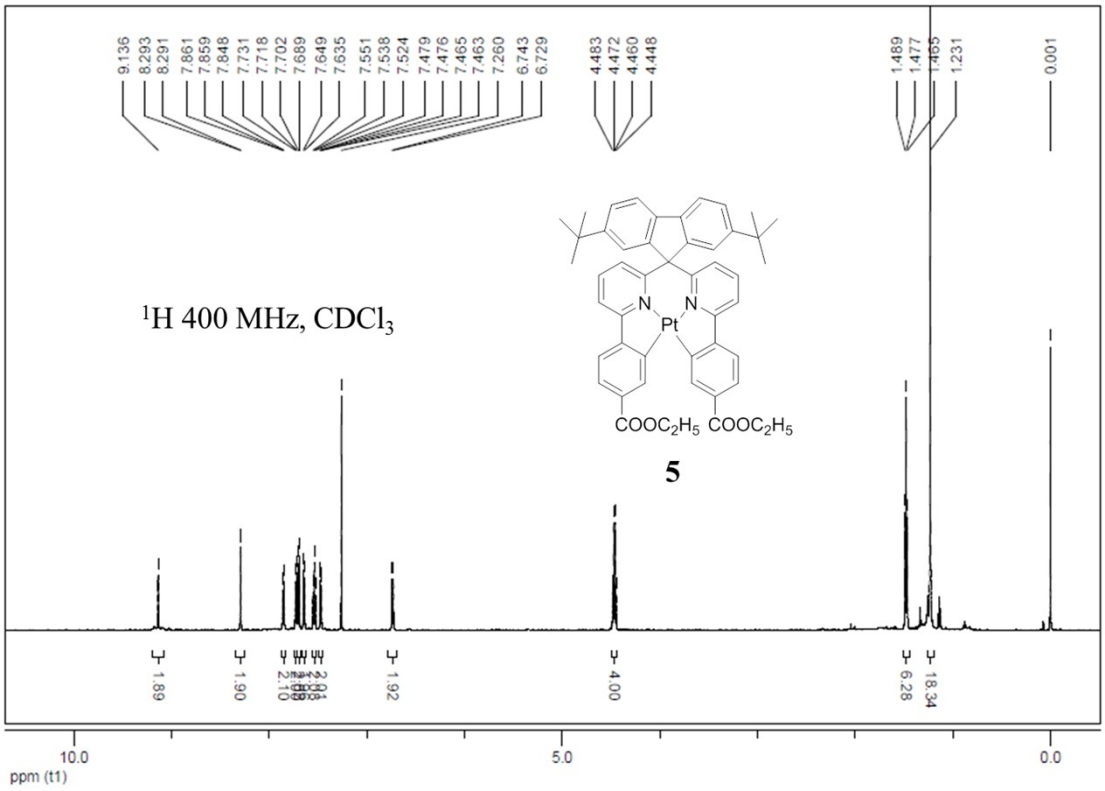
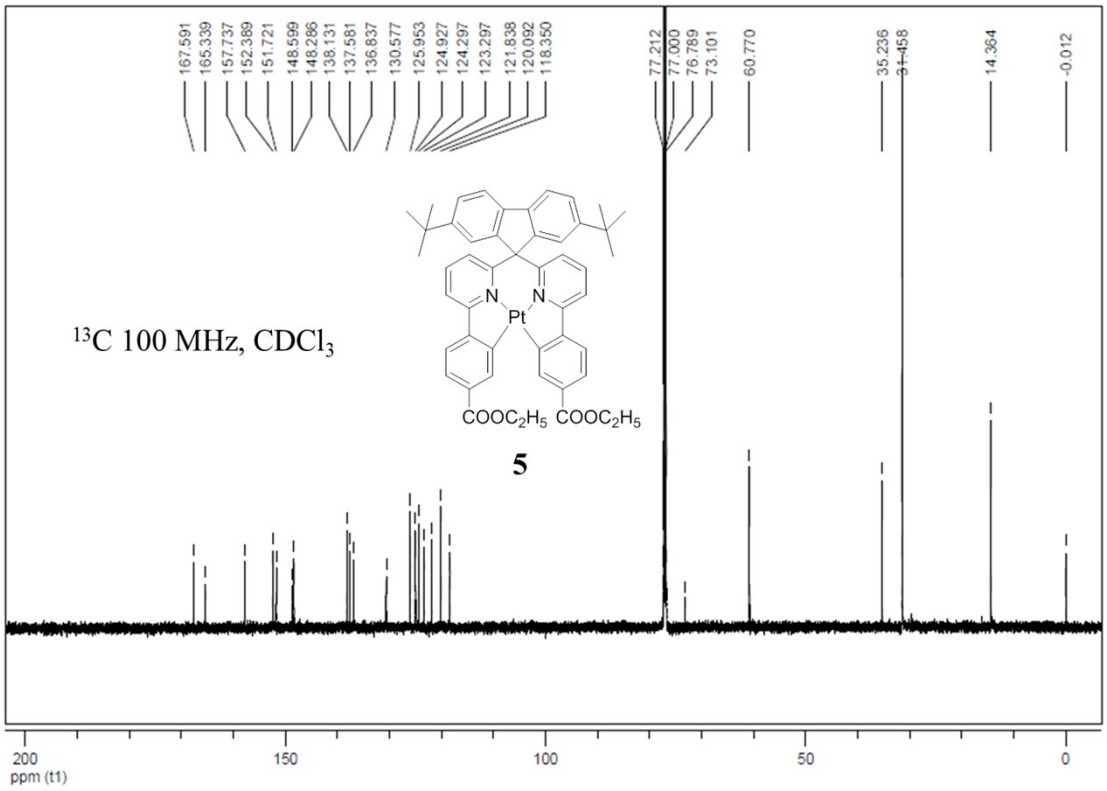
m/z
800

Fig. S3 ^{1}H NMR, ^{13}C NMR and ESI-MS spectra of intermediates **5.**





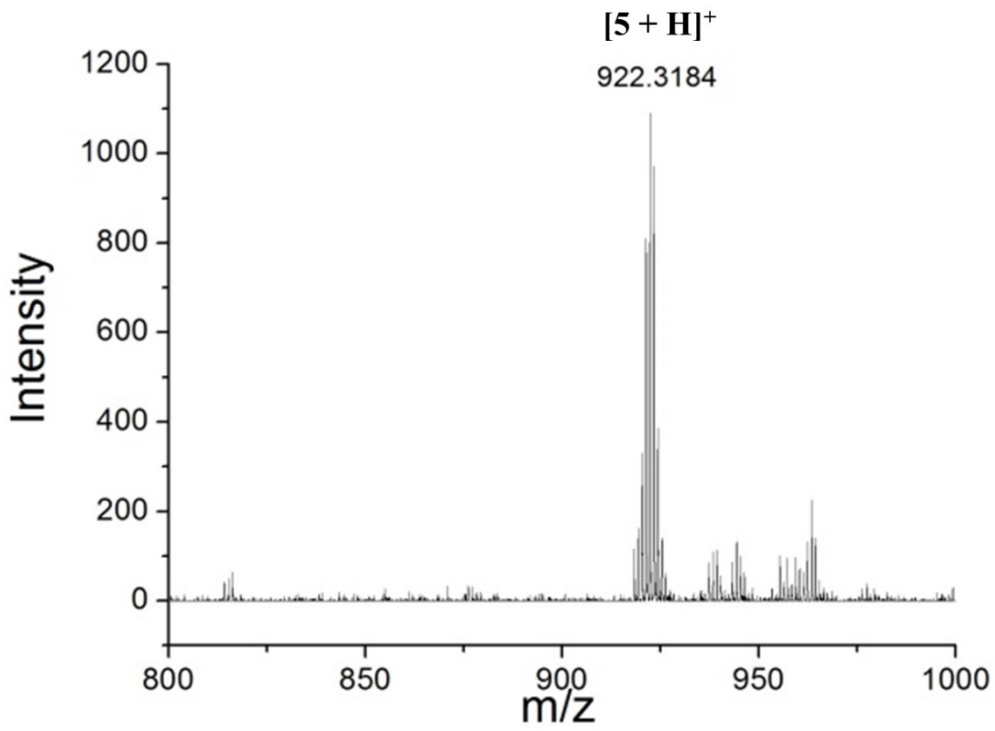
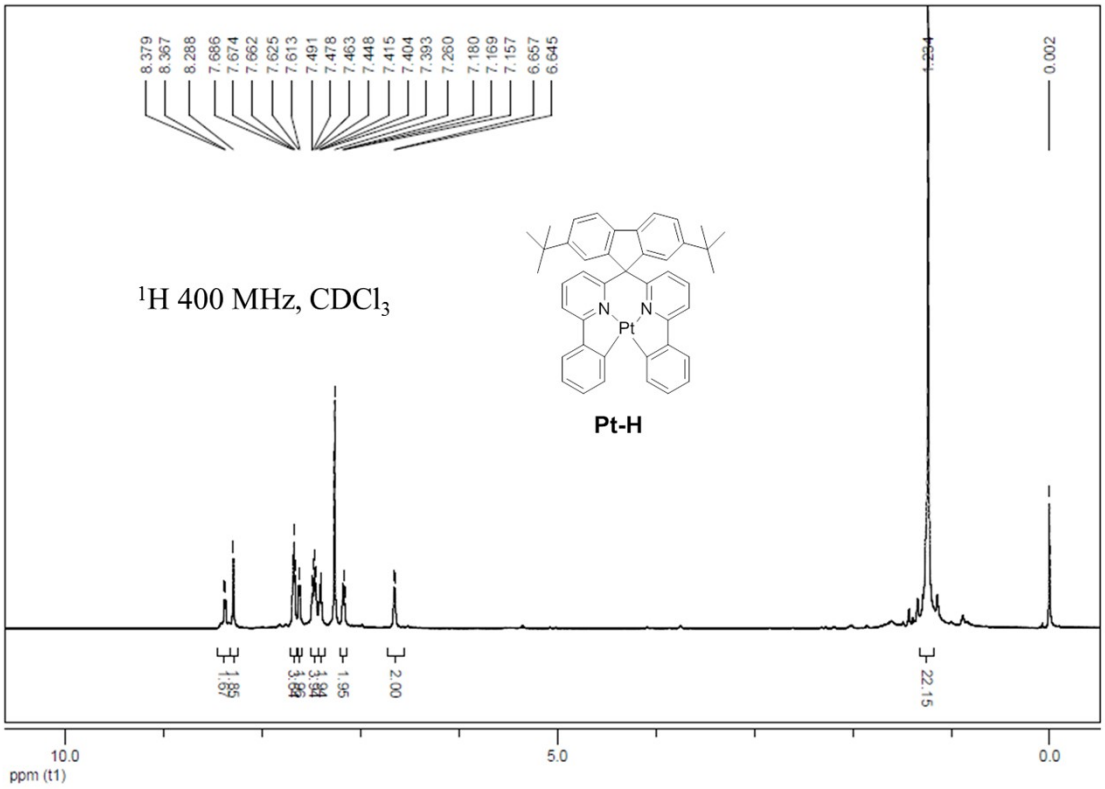
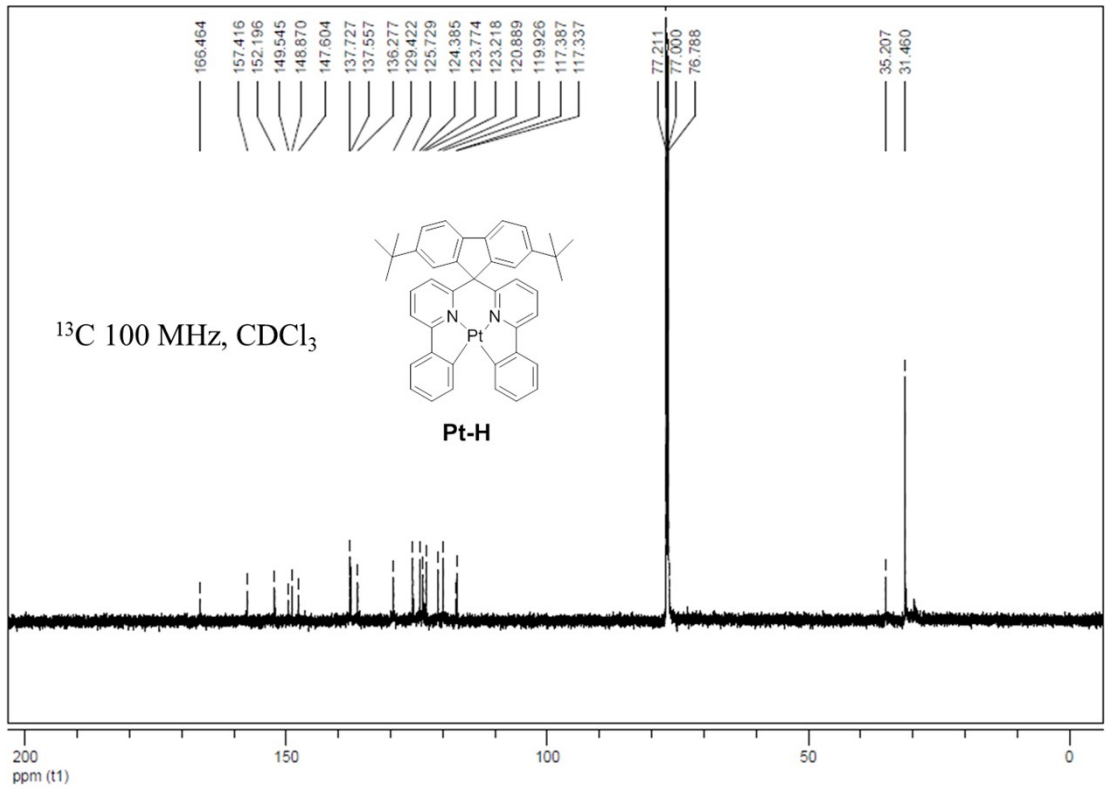


Fig. S4 ^{1}H NMR, ^{13}C NMR and ESI-HRMS spectra of **Pt-H.**

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157.416
152.196
149.545
148.870
147.604
137.727
137.557
136.277
129.422
125.729
124.385
123.774
123.218
120.889
119.926
117.387
117.337
77.211
77.000
76.788
35.207
31.460
^{13}C 100 MHz, CDCl$_3$
N
Pt
N
Pt-H
200
150
100
50
0
ppm (t1)

[Pt-H + H]$^+$

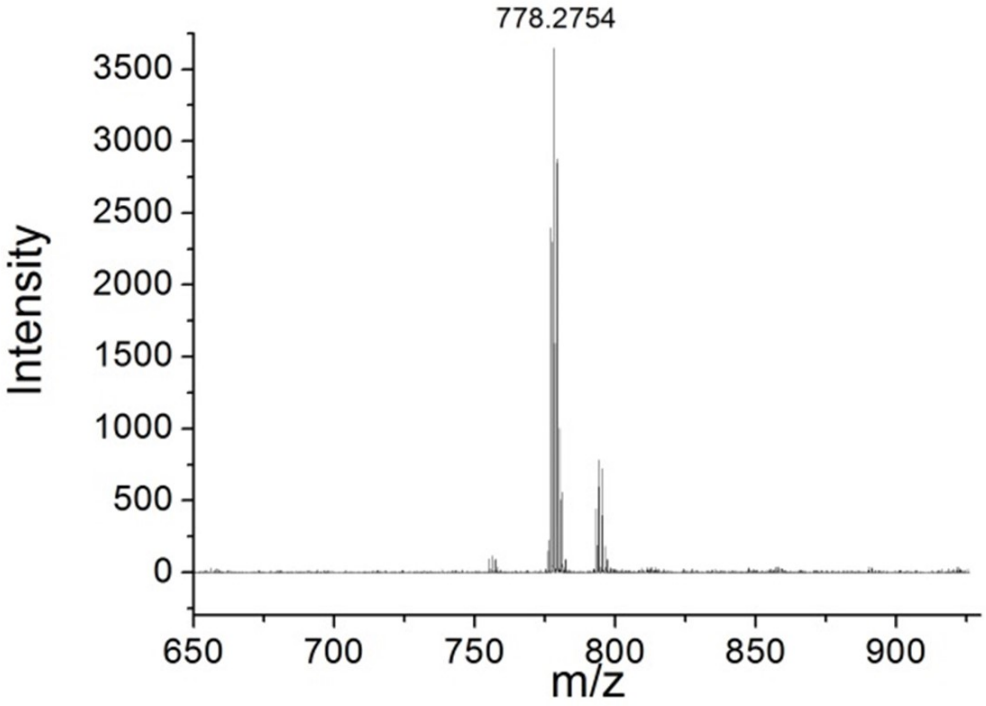
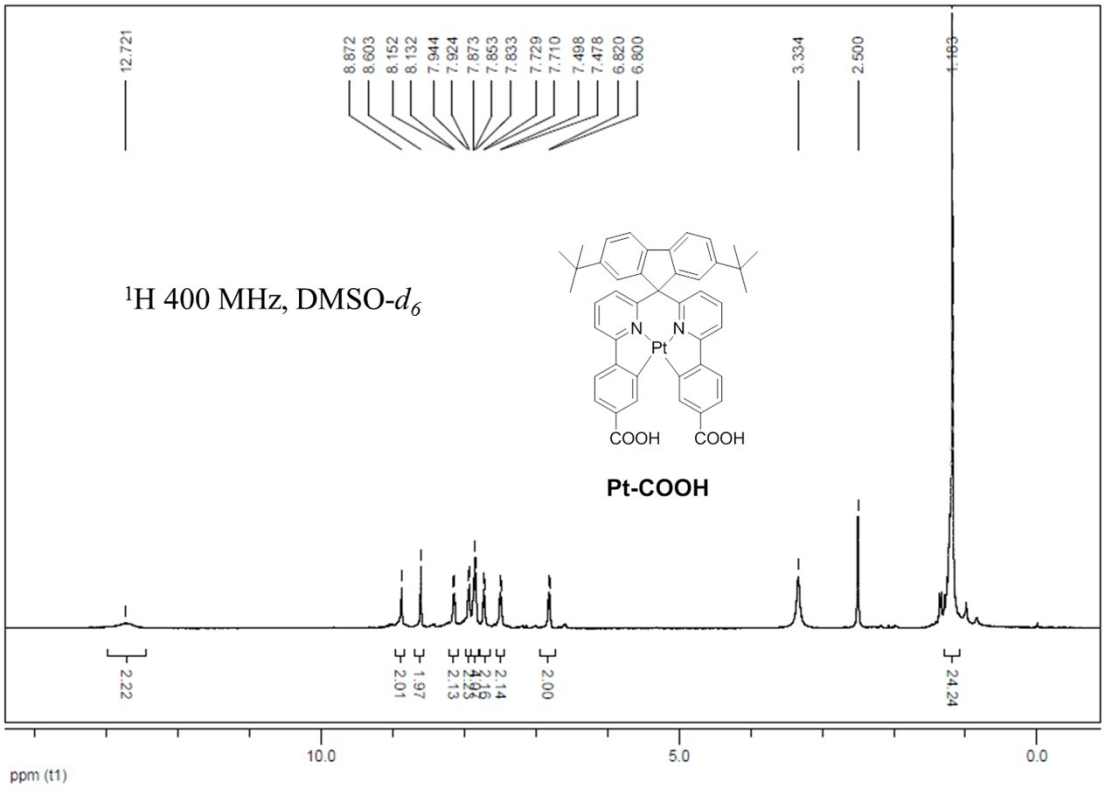
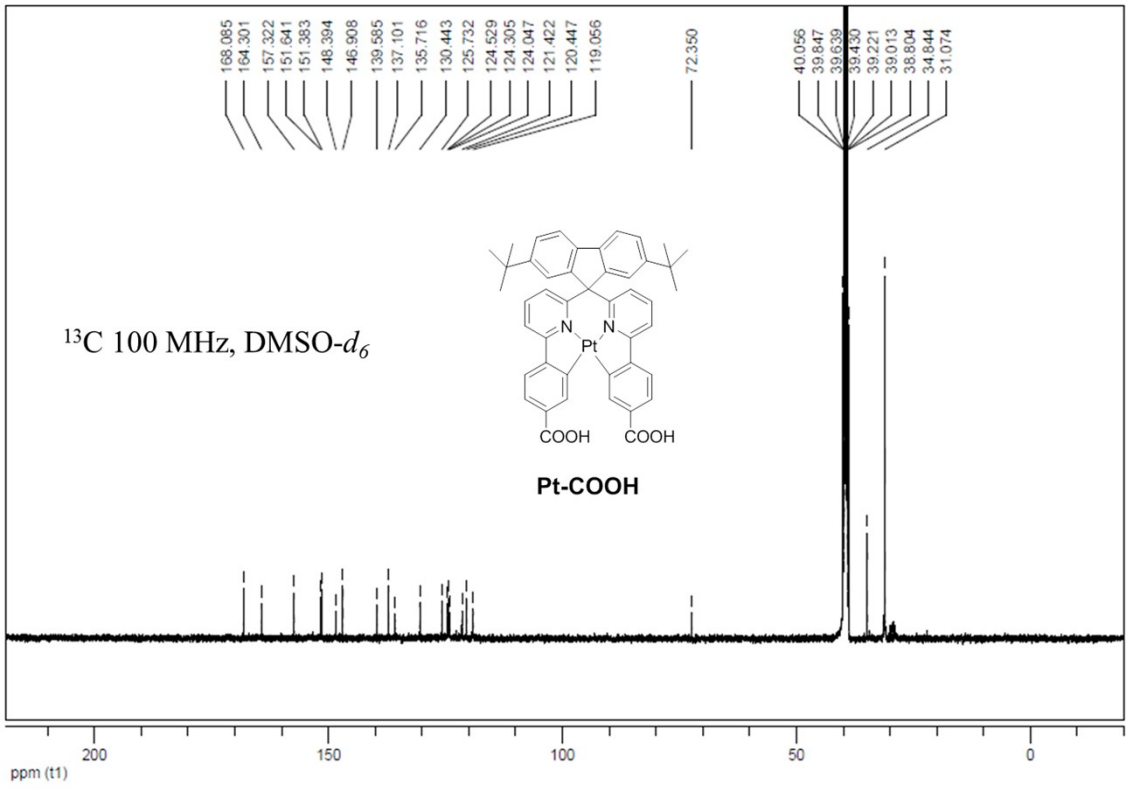

778.2754
Intensity
3500
3000
2500
2000
1500
1000
500
0
650
700
750
800
850
900
m/z

Fig. S5 ^{1}H NMR, ^{13}C NMR and ESI-HRMS spectra of **Pt-COOH**.





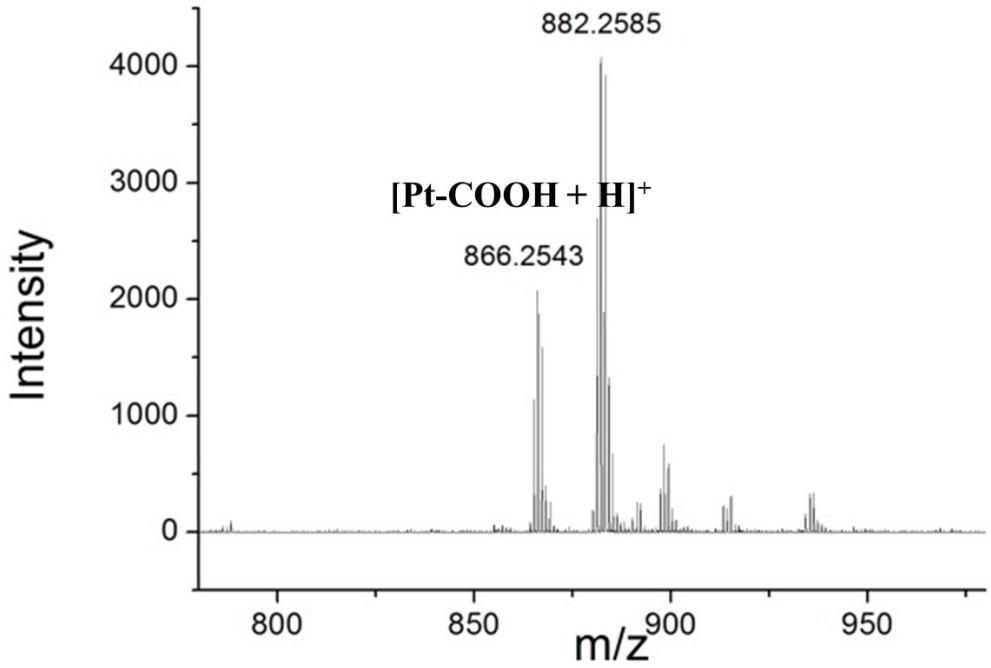


Fig. S6 Absorption spectra in DMSO and Cyclic voltammogram in 0.1 M *n*-NBu_4PF_6 solutions in DMSO at the scan rates of 100 mV/s.

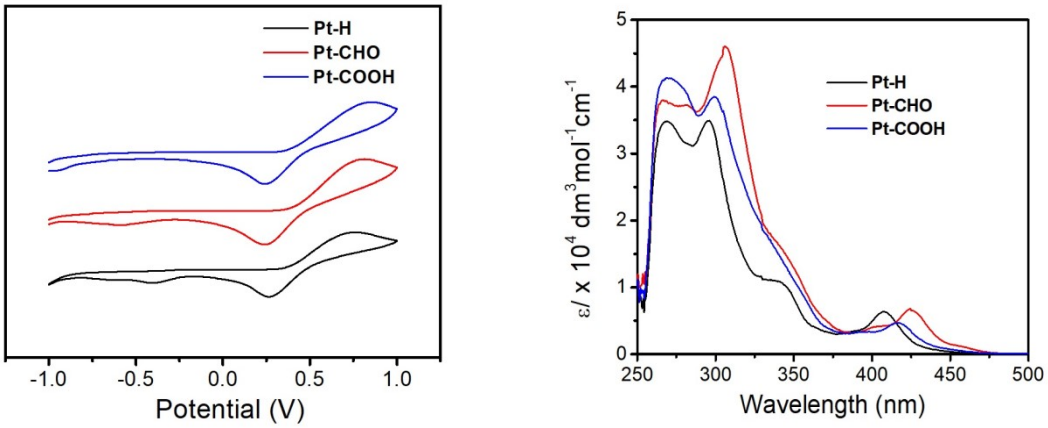


Fig. S7 Bright, luminescence, and merged photos of RAW264.7 cells treated with different concentrations of **Pt-H.**

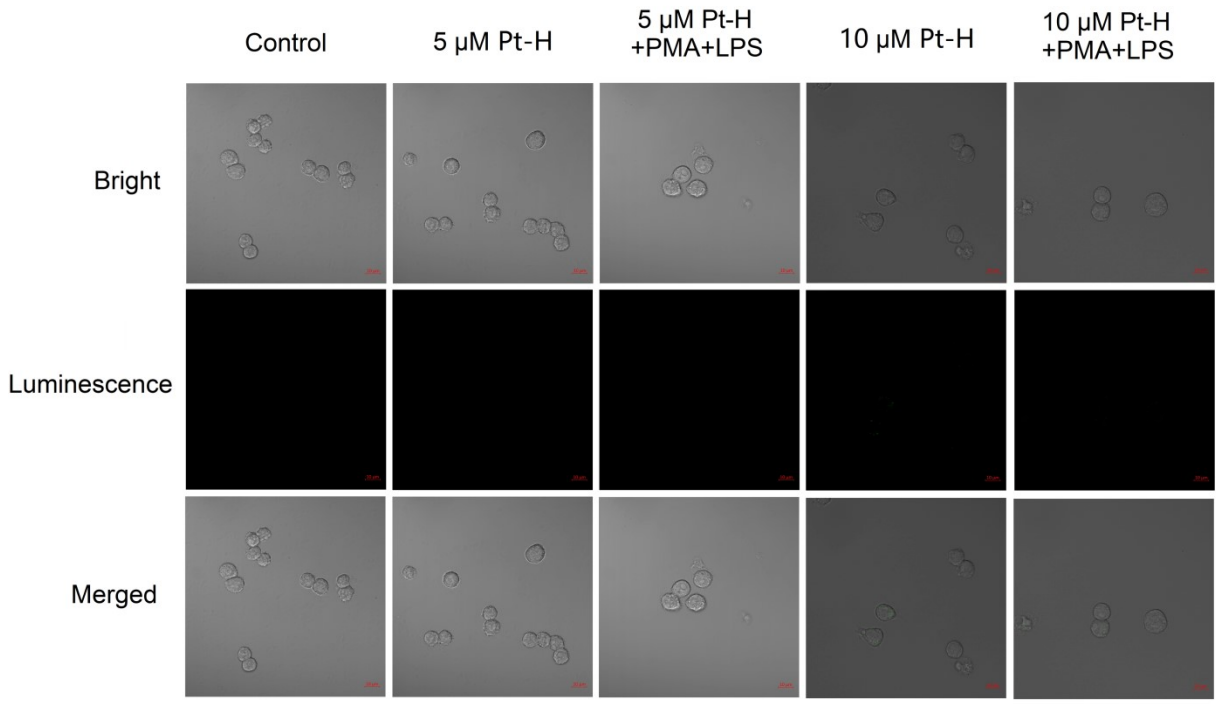


Table S1 Electrochemical data of the probes

complexes	E_{ox}[a] (V)	E_{red}[b] (V)	E_g[c] (eV)
Pt-H	0.35	−2.46	2.81
Pt-CHO	0.36	−2.25	2.61
Pt-COOH	0.36	−2.40	2.76

[a] E_{ox} was determined from onset potentials using Ag/AgCl as the reference electrode. [b] $E_{red} = E_{ox}$-E_g. [c] optical band gap.

Table S2 The structure coordinates of the probes and the oxidative products.

Pt-H

C	1.477012	-2.238782	-2.993474
C	0.168082	-2.684401	-2.968520
C	-0.686096	-2.227784	-1.965172
N	-0.230189	-1.357056	-1.022766
C	1.034823	-0.906049	-1.036336
C	1.917424	-1.344332	-2.027471
C	1.500898	0.215743	-0.081021
C	0.964181	0.303811	1.364681
N	-0.357901	0.224484	1.587199
C	-0.901495	0.517118	2.798627
C	-0.075798	0.850122	3.872657
C	1.292162	0.897528	3.675508
C	1.820419	0.641708	2.414470
C	-2.089178	-2.619188	-1.819253
C	-2.365430	0.482769	2.831330
C	-2.681338	-3.579283	-2.650123
C	-3.994515	-3.973084	-2.440560
C	-4.707526	-3.419262	-1.378512
C	-4.120582	-2.462663	-0.553717
C	-2.811196	-2.006954	-0.758190
C	-3.004295	-0.027688	1.667932
C	-4.396674	0.115787	1.609972
C	-5.125634	0.659820	2.665788
C	-4.481873	1.090664	3.825043
C	-3.098169	1.013873	3.899546
C	1.175147	1.565389	-0.759587
C	3.028690	0.268581	-0.063566
C	3.907831	-0.699374	0.408269
C	5.290076	-0.486254	0.349454
C	5.743299	0.726518	-0.200416
C	4.871640	1.695871	-0.679948
C	3.497679	1.465378	-0.612919
C	2.356612	2.268093	-1.043740
C	2.280674	3.514759	-1.651184
C	1.028502	4.041897	-1.967700
C	-0.157747	3.350743	-1.693267
C	-0.063396	2.089947	-1.078584
C	6.304427	-1.514807	0.855036
C	5.629254	-2.768723	1.417113
C	7.219913	-1.941867	-0.304258
C	7.155485	-0.886768	1.971118
C	-1.541845	3.908959	-2.028824

C	-1.467750	5.282003	-2.701709
C	-2.264146	2.941783	-2.981976
C	-2.359725	4.047575	-0.733353
Pt	-1.707396	-0.745139	0.327648
H	2.158727	-2.577865	-3.768648
H	-0.195152	-3.372599	-3.722455
H	2.933840	-0.975969	-2.051157
H	-0.504974	1.055495	4.846636
H	1.956946	1.146457	4.498171
H	2.885776	0.719158	2.248387
H	-2.118258	-4.037295	-3.459501
H	-4.694905	-2.079284	0.282277
H	-4.928193	-0.188479	0.713606
H	-2.592899	1.396475	4.783311
H	3.509611	-1.621063	0.821962
H	6.811799	0.917514	-0.258500
H	5.261671	2.618158	-1.102881
H	3.181022	4.079312	-1.881364
H	0.986461	5.016932	-2.441723
H	-0.962010	1.519910	-0.847107
H	6.393927	-3.472120	1.764983
H	4.982075	-2.536829	2.270849
H	5.028020	-3.283881	0.659125
H	7.957077	-2.674921	0.045086
H	7.768365	-1.092949	-0.726052
H	6.639690	-2.401419	-1.112413
H	6.528662	-0.580490	2.816301
H	7.892597	-1.610819	2.338846
H	7.701316	-0.004061	1.621453
H	-2.480917	5.635873	-2.922852
H	-0.991773	6.028731	-2.055252
H	-0.917390	5.243647	-3.649254
H	-3.258688	3.331639	-3.230940
H	-2.398186	1.951854	-2.533292
H	-1.702814	2.818329	-3.915385
H	-1.869147	4.732298	-0.031892
H	-3.356433	4.446523	-0.958331
H	-2.492832	3.084573	-0.228973
H	-5.051482	1.507400	4.651107
H	-4.451829	-4.717458	-3.086537
H	-5.728750	-3.741294	-1.186225
H	-6.206377	0.752316	2.582118

Pt-H-2

C	1.365828	-0.992356	-3.577710
C	0.091172	-1.534842	-3.632257
C	-0.706860	-1.490068	-2.493916
N	-0.237657	-0.921388	-1.353644
C	0.986763	-0.396840	-1.273657
C	1.820910	-0.426586	-2.399218
C	1.530308	0.349729	-0.037356
C	0.900068	0.238968	1.365975
N	-0.421112	0.132878	1.541492
C	-0.993794	0.189980	2.768425
C	-0.208439	0.378705	3.902052
C	1.162543	0.494309	3.747943
C	1.723971	0.428535	2.481156
C	-2.062227	-2.044330	-2.401467
C	-2.455143	0.059396	2.775930
C	-2.626357	-2.817162	-3.422661
C	-3.873253	-3.404573	-3.255466
C	-4.548797	-3.243318	-2.049453
C	-3.995072	-2.469226	-1.029248
C	-2.768456	-1.828088	-1.195594
C	-3.067485	-0.351528	1.569855
C	-4.459673	-0.328747	1.500678
C	-5.230760	0.020075	2.610466
C	-4.619261	0.367880	3.811454
C	-3.232703	0.400346	3.887515
C	1.538214	1.853744	-0.376224
C	3.031377	0.071421	0.065419
C	3.647077	-1.144777	0.326874
C	5.043522	-1.220967	0.397462
C	5.776463	-0.037805	0.195933
C	5.165033	1.182089	-0.069521
C	3.773403	1.241304	-0.137010
C	2.852977	2.344443	-0.408383
C	3.064394	3.689049	-0.687398
C	1.963536	4.511266	-0.933627
C	0.650497	4.023504	-0.912977
C	0.446375	2.662753	-0.623243
C	5.782340	-2.530454	0.683397
C	4.822923	-3.708576	0.872112
C	6.717708	-2.856319	-0.492730
C	6.613570	-2.377298	1.967904
C	-0.568481	4.900746	-1.201275
C	-0.189615	6.358467	-1.472089
C	-1.303387	4.345857	-2.433834

C	-1.519205	4.859027	0.007093
Pt	-1.737805	-0.738062	0.126580
H	2.005918	-1.005648	-4.455435
H	-0.283678	-1.973710	-4.549271
H	2.812144	0.005643	-2.344915
H	-0.662761	0.406787	4.885606
H	1.802466	0.632136	4.615108
H	2.793550	0.529091	2.355685
H	-2.085479	-2.984307	-4.350192
H	-5.510362	-3.727004	-1.894985
H	-4.528422	-2.384429	-0.088448
H	-4.962575	-0.571986	0.569782
H	-6.315232	0.025375	2.530730
H	-2.759697	0.723029	4.811402
H	3.033484	-2.027746	0.478948
H	6.861876	-0.070676	0.245844
H	5.769268	2.072734	-0.222689
H	4.069408	4.103137	-0.719158
H	2.145152	5.558809	-1.151356
H	-0.558638	2.234766	-0.609923
H	5.397166	-4.619855	1.073385
H	4.144133	-3.552553	1.718251
H	4.218056	-3.890739	-0.023492
H	7.258501	-3.790645	-0.299093
H	7.461201	-2.068507	-0.654542
H	6.149707	-2.978082	-1.421920
H	5.969791	-2.152869	2.825863
H	7.154569	-3.306950	2.182326
H	7.352766	-1.573488	1.883331
H	-1.096116	6.942481	-1.667358
H	0.319202	6.814852	-0.614525
H	0.459734	6.455454	-2.350290
H	-2.185188	4.960889	-2.653743
H	-1.639577	3.316357	-2.270349
H	-0.652374	4.358258	-3.315896
H	-1.023773	5.231676	0.911268
H	-2.397917	5.487661	-0.183803
H	-1.870389	3.840649	0.203385
H	-5.218068	0.638249	4.676562
H	-4.303299	-4.004022	-4.052828
O	-1.089638	-2.421111	1.043607
H	-1.762134	-3.097193	0.881732
O	-2.202102	1.011090	-0.805965
H	-3.120319	1.204530	-0.572242

Pt-CHO

C	1.963631	2.860077	2.399876
C	0.628464	3.223326	2.370868
C	-0.247951	2.515136	1.552106
N	0.205453	1.484395	0.787479
C	1.495305	1.111442	0.808204
C	2.402372	1.799980	1.620398
C	1.980145	-0.164282	0.085280
C	1.368833	-0.595759	-1.265167
N	0.034760	-0.626716	-1.413748
C	-0.552882	-1.206453	-2.493855
C	0.230098	-1.734397	-3.519172
C	1.607730	-1.675969	-3.405562
C	2.185381	-1.121887	-2.269082
C	-1.683350	2.789985	1.429810
C	-2.017396	-1.245810	-2.439962
C	-2.285887	3.870048	2.088973
C	-3.634122	4.129395	1.909095
C	-4.376218	3.317323	1.047866
C	-3.769479	2.242867	0.389857
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C	-2.620977	-0.522037	-1.376307
C	-3.998365	-0.707785	-1.212045
C	-4.750150	-1.499379	-2.083813
C	-4.137613	-2.148077	-3.161796
C	-2.770887	-2.028661	-3.328899
C	1.784883	-1.348432	1.059633
C	3.504694	-0.137631	-0.028551
C	4.287568	0.748521	-0.759644
C	5.682139	0.626760	-0.754790
C	6.246425	-0.410357	0.009988
C	5.471303	-1.295858	0.747774
C	4.083400	-1.158676	0.730765
C	3.025614	-1.907559	1.403402
C	3.068275	-2.994448	2.266954
C	1.874398	-3.506425	2.775405
C	0.630196	-2.956583	2.443870
C	0.604467	-1.856194	1.569112
C	6.594729	1.570946	-1.540921
C	5.806386	2.633656	-2.311106
C	7.544940	2.289108	-0.568407
C	7.419930	0.758121	-2.552278
C	-0.691225	-3.501018	2.989135

C	-0.487006	-4.699136	3.919809
C	-1.410415	-2.393121	3.777285
C	-1.580098	-3.945721	1.815102
Pt	-1.299787	0.523252	-0.300996
H	2.665499	3.393808	3.034435
H	0.266362	4.040664	2.982883
H	3.439899	1.496528	1.650853
H	-0.237467	-2.171858	-4.393562
H	2.240893	-2.072993	-4.194082
H	3.260746	-1.111719	-2.159170
H	-1.706201	4.521195	2.737384
H	-4.391325	1.676053	-0.293095
H	-4.513211	-0.242043	-0.375622
H	-2.286788	-2.568748	-4.138640
H	3.805641	1.534347	-1.333771
H	7.326796	-0.527465	0.031435
H	5.946300	-2.081235	1.330028
H	4.016055	-3.446728	2.548571
H	1.925134	-4.356156	3.447997
H	-0.342663	-1.399834	1.285286
H	6.501365	3.282118	-2.855928
H	5.127909	2.186754	-3.046975
H	5.217443	3.271205	-1.641631
H	8.210562	2.964797	-1.118847
H	8.171946	1.583316	-0.013426
H	6.983290	2.884269	0.160513
H	6.767534	0.241821	-3.265612
H	8.085332	1.421130	-3.118171
H	8.042099	0.003318	-2.059835
H	-1.459677	-5.051425	4.280593
H	-0.002902	-5.537823	3.405806
H	0.115119	-4.437111	4.797821
H	-2.361148	-2.769709	4.173611
H	-1.633551	-1.525144	3.147709
H	-0.800044	-2.052444	4.621644
H	-1.093468	-4.736413	1.232539
H	-2.532804	-4.337423	2.191515
H	-1.806834	-3.116340	1.136631
H	-4.747327	-2.750653	-3.828144
H	-4.110647	4.963624	2.419745
C	-5.808183	3.603003	0.833757
O	-6.546941	2.955211	0.123614
H	-6.191563	4.488289	1.390441
C	-6.201825	-1.653799	-1.860853

O	-6.935689	-2.324671	-2.555782
H	-6.599496	-1.096322	-0.984824

Pt-CHO-2

C	1.856759	-1.460802	-3.403613
C	0.531572	-1.865015	-3.475638
C	-0.307802	-1.603055	-2.399718
N	0.166117	-0.964304	-1.299239
C	1.436501	-0.569656	-1.202647
C	2.314170	-0.816812	-2.268380
C	2.006357	0.246661	-0.025385
C	1.301092	0.377826	1.338669
N	-0.029570	0.419916	1.451874
C	-0.644490	0.685410	2.630200
C	0.104213	0.937900	3.774784
C	1.486162	0.902886	3.684652
C	2.090668	0.626865	2.468306
C	-1.723901	-1.986176	-2.334847
C	-2.111249	0.697731	2.574004
C	-2.323748	-2.787225	-3.313762
C	-3.640738	-3.196242	-3.172262
C	-4.355819	-2.827488	-2.032854
C	-3.756641	-2.025763	-1.053037
C	-2.457148	-1.559982	-1.198739
C	-2.709937	0.213265	1.388208
C	-4.088635	0.355366	1.255108
C	-4.866846	0.894788	2.285013
C	-4.267308	1.319780	3.473184
C	-2.893518	1.231623	3.608561
C	2.216701	1.688247	-0.530376
C	3.454672	-0.193145	0.200817
C	3.900162	-1.432967	0.637774
C	5.271470	-1.664722	0.801762
C	6.154623	-0.609778	0.510239
C	5.713663	0.632739	0.069536
C	4.345014	0.847919	-0.089060
C	3.582682	2.011596	-0.539465
C	3.971856	3.278565	-0.956495
C	2.993893	4.189774	-1.358785
C	1.630387	3.867978	-1.360200
C	1.245842	2.585283	-0.931136
C	5.827239	-3.007617	1.281290
C	4.720773	-4.032100	1.546118
C	6.768078	-3.582392	0.209408

C	6.610936	-2.797809	2.587540
C	0.544823	4.844092	-1.815397
C	1.115417	6.202713	-2.228270
C	-0.200873	4.237948	-3.016945
C	-0.453586	5.062297	-0.665916
Pt	-1.367441	-0.460441	0.065869
H	2.532521	-1.643306	-4.234216
H	0.154473	-2.362767	-4.360945
H	3.344024	-0.489479	-2.200836
H	-0.386454	1.133232	4.720939
H	2.098296	1.087228	4.562934
H	3.169343	0.608585	2.389765
H	-1.760655	-3.112124	-4.183685
H	-4.348209	-1.801620	-0.172305
H	-4.589078	0.059318	0.336702
H	-2.424958	1.606353	4.514378
H	3.175152	-2.212281	0.853208
H	7.223850	-0.764562	0.629868
H	6.431001	1.420154	-0.147423
H	5.020843	3.564257	-0.975564
H	3.314105	5.174728	-1.682691
H	0.196009	2.284155	-0.927915
H	5.167065	-4.973252	1.886029
H	4.028259	-3.695158	2.325856
H	4.140258	-4.250068	0.642392
H	7.178776	-4.543226	0.542304
H	7.610676	-2.913758	0.003152
H	6.233056	-3.749104	-0.732311
H	5.961334	-2.396510	3.373585
H	7.021758	-3.751626	2.939871
H	7.447512	-2.103237	2.455814
H	0.298800	6.863418	-2.540210
H	1.640139	6.694579	-1.400503
H	1.808649	6.115187	-3.073256
H	-0.988292	4.923292	-3.354741
H	-0.670716	3.283068	-2.757874
H	0.483257	4.066975	-3.856396
H	0.045903	5.480031	0.215975
H	-1.238024	5.763208	-0.976987
H	-0.937655	4.124570	-0.373674
H	-4.893792	1.733120	4.257727
H	-4.109573	-3.816886	-3.932812
O	-0.953295	-2.099951	1.174586
H	-1.748474	-2.650636	1.168474

O	-1.578663	1.217665	-1.066054
H	-2.478826	1.538064	-0.917206
C	-5.747849	-3.284481	-1.856585
O	-6.450567	-3.003805	-0.909491
H	-6.133780	-3.926985	-2.679264
C	-6.328342	1.019750	2.108046
O	-7.080303	1.482861	2.938517
H	-6.713158	0.649353	1.132860

Pt-COOH

C	2.073884	3.109015	2.108866
C	0.724135	3.407511	2.045353
C	-0.116909	2.584570	1.299458
N	0.385567	1.505860	0.639034
C	1.690648	1.194981	0.695332
C	2.563114	1.998854	1.435904
C	2.233037	-0.122633	0.099015
C	1.648036	-0.704676	-1.206100
N	0.317173	-0.808508	-1.351296
C	-0.239645	-1.509961	-2.373999
C	0.570227	-2.093822	-3.346794
C	1.943390	-1.964357	-3.238700
C	2.491234	-1.283704	-2.157377
C	-1.561871	2.781922	1.150202
C	-1.700891	-1.610613	-2.315363
C	-2.215028	3.895019	1.696611
C	-3.570641	4.083966	1.491992
C	-4.272877	3.158346	0.713823
C	-3.620384	2.048426	0.171387
C	-2.260371	1.804244	0.389848
C	-2.340304	-0.824967	-1.318688
C	-3.705909	-1.057150	-1.123524
C	-4.419636	-1.956948	-1.920714
C	-3.779229	-2.663925	-2.942440
C	-2.417958	-2.499509	-3.127466
C	2.082007	-1.215691	1.181436
C	3.755692	-0.042690	-0.013920
C	4.504980	0.802509	-0.824348
C	5.903375	0.741870	-0.804744
C	6.506407	-0.192374	0.056824
C	5.764837	-1.036072	0.873921
C	4.372457	-0.960954	0.840688
C	3.343023	-1.686391	1.579703
C	3.426261	-2.682364	2.544060

C	2.251993	-3.192853	3.097667
C	0.987855	-2.730240	2.712622
C	0.921056	-1.721377	1.735760
C	6.779498	1.645999	-1.674855
C	5.950822	2.591971	-2.548090
C	7.687930	2.497639	-0.772626
C	7.649464	0.778290	-2.599323
C	-0.312813	-3.275924	3.304512
C	-0.063037	-4.359305	4.356833
C	-1.091813	-2.127685	3.968067
C	-1.167057	-3.882507	2.178054
Pt	-1.072666	0.377556	-0.349571
H	2.748702	3.732853	2.688271
H	0.322975	4.263234	2.575033
H	3.613067	1.746889	1.495476
H	0.125649	-2.629938	-4.177227
H	2.596903	-2.403392	-3.987386
H	3.564637	-1.216277	-2.048470
H	-1.667810	4.631921	2.278152
H	-4.213494	1.385879	-0.447494
H	-4.237814	-0.544328	-0.331080
H	-1.913932	-3.087238	-3.890381
H	3.993580	1.508878	-1.471544
H	7.590666	-0.260157	0.092090
H	6.269086	-1.741167	1.529718
H	4.390568	-3.064848	2.869685
H	2.334373	-3.970736	3.849456
H	-0.042588	-1.334198	1.408013
H	6.620521	3.215019	-3.151144
H	5.298980	2.045052	-3.239122
H	5.328450	3.264456	-1.946502
H	8.327264	3.146564	-1.383234
H	8.341054	1.878173	-0.148861
H	7.093558	3.134258	-0.107487
H	7.027449	0.165130	-3.261271
H	8.287984	1.413765	-3.224705
H	8.302039	0.104913	-2.033641
H	-1.021964	-4.715170	4.749540
H	0.461879	-5.224818	3.935701
H	0.520039	-3.979522	5.204152
H	-2.027497	-2.506497	4.396774
H	-1.350188	-1.342152	3.250072
H	-0.506954	-1.671472	4.775161
H	-0.637149	-4.704918	1.683779

H	-2.104136	-4.278511	2.587837
H	-1.425800	-3.139791	1.415819
H	-4.359601	-3.346874	-3.554151
H	-4.081712	4.942733	1.913023
C	-5.718099	3.321133	0.428905
O	-6.389727	2.565055	-0.238256
O	-6.248186	4.426557	0.997301
H	-7.185237	4.418837	0.738373
C	-5.870587	-2.195084	-1.728426
O	-6.549437	-2.923400	-2.421645
O	-6.385452	-1.513024	-0.689187
H	-7.334234	-1.723806	-0.681839

Pt-COOH-2

C	1.955927	-1.866559	-3.227255
C	0.612559	-2.212526	-3.233103
C	-0.191449	-1.793588	-2.179768
N	0.334547	-1.060937	-1.165078
C	1.623568	-0.719884	-1.132608
C	2.466597	-1.124187	-2.177680
C	2.254176	0.190971	-0.059874
C	1.582138	0.501260	1.292129
N	0.257584	0.628872	1.414801
C	-0.322200	1.048987	2.565466
C	0.458092	1.378423	3.668741
C	1.834264	1.257416	3.567608
C	2.402751	0.822394	2.380429
C	-1.621810	-2.098353	-2.049961
C	-1.786811	1.135911	2.523942
C	-2.277691	-2.980137	-2.917178
C	-3.607007	-3.313632	-2.712794
C	-4.282040	-2.780301	-1.613460
C	-3.631820	-1.893829	-0.747696
C	-2.313388	-1.509569	-0.964953
C	-2.430491	0.562037	1.403546
C	-3.799127	0.766223	1.257554
C	-4.531420	1.457086	2.230437
C	-3.894580	1.967280	3.362363
C	-2.524511	1.818270	3.498842
C	2.521313	1.558653	-0.719433
C	3.684617	-0.291232	0.191496
C	4.080596	-1.498286	0.750608
C	5.442513	-1.777399	0.918748
C	6.367941	-0.802495	0.505273

C	5.976536	0.406754	-0.057921
C	4.616538	0.669556	-0.219375
C	3.900287	1.814136	-0.780680
C	4.339738	3.010065	-1.334919
C	3.397600	3.918950	-1.819525
C	2.021022	3.663560	-1.769531
C	1.585680	2.453418	-1.200940
C	5.943858	-3.088224	1.529132
C	4.795685	-4.024885	1.914568
C	6.836964	-3.816653	0.511218
C	6.760011	-2.781970	2.795810
C	0.973517	4.635120	-2.314636
C	1.597857	5.915915	-2.872944
C	0.185781	3.940731	-3.439136
C	0.000778	5.017237	-1.186054
Pt	-1.149060	-0.327867	0.151852
H	2.604990	-2.171359	-4.043212
H	0.193852	-2.785800	-4.051538
H	3.511684	-0.841413	-2.163062
H	-0.006102	1.698503	4.594135
H	2.470228	1.498183	4.414805
H	3.477404	0.736002	2.292770
H	-1.747668	-3.431139	-3.751031
H	-4.195160	-1.533240	0.105439
H	-4.324911	0.402042	0.382694
H	-2.027654	2.261967	4.357069
H	3.324256	-2.214805	1.057006
H	7.430989	-0.995050	0.625461
H	6.725305	1.131672	-0.367058
H	5.400253	3.242015	-1.397562
H	3.756804	4.847856	-2.250451
H	0.523256	2.205087	-1.152179
H	5.203637	-4.946416	2.344573
H	4.134413	-3.575792	2.664311
H	4.188697	-4.306644	1.046591
H	7.207988	-4.756494	0.937603
H	7.706169	-3.214931	0.224838
H	6.277542	-4.054198	-0.400632
H	6.144466	-2.269164	3.543491
H	7.131139	-3.712847	3.241315
H	7.626198	-2.147005	2.580940
H	0.806896	6.577172	-3.244249
H	2.155957	6.466607	-2.106265
H	2.274191	5.709493	-3.710940

H	-0.575190	4.621733	-3.840506
H	-0.321970	3.040695	-3.076239
H	0.850437	3.651634	-4.261712
H	0.529991	5.500612	-0.356550
H	-0.754875	5.717859	-1.562341
H	-0.521804	4.138401	-0.794124
H	-4.485235	2.494197	4.104624
H	-4.115056	-3.997545	-3.383703
O	-0.799973	-1.847846	1.439675
H	-1.616420	-2.364184	1.488887
O	-1.298130	1.219872	-1.161131
H	-2.193608	1.572658	-1.066817
C	-5.690008	-3.130619	-1.311723
O	-6.323915	-2.711653	-0.368112
O	-6.224737	-3.986118	-2.207751
H	-7.135953	-4.138074	-1.904496
C	-5.993070	1.672844	2.103592
O	-6.683637	2.222960	2.934296
O	-6.498162	1.190584	0.953495
H	-7.453837	1.364229	0.991682

Table S3 The excited states analysis of the probes and the oxidative products.

Pt-H

Excited State 1:	f=0.0039	<S**2>=0.000	415.87nm	2.9813eV	Singlet-A
Excited State 2:	f=0.0457	<S**2>=0.000	385.14nm	3.2192eV	Singlet-A
Excited State 3:	f=0.0062	<S**2>=0.000	372.69nm	3.3267eV	Singlet-A
Excited State 4:	f=0.0846	<S**2>=0.000	357.49nm	3.4682eV	Singlet-A
Excited State 5:	f=0.0040	<S**2>=0.000	342.43nm	3.6207eV	Singlet-A
Excited State 6:	f=0.0222	<S**2>=0.000	337.10nm	3.6780eV	Singlet-A
Excited State 7:	f=0.0212	<S**2>=0.000	334.93nm	3.7018eV	Singlet-A
Excited State 8:	f=0.0089	<S**2>=0.000	322.94nm	3.8392eV	Singlet-A
Excited State 9:	f=0.0074	<S**2>=0.000	320.43nm	3.8693eV	Singlet-A
Excited State 10:	f=0.0141	<S**2>=0.000	317.21nm	3.9085eV	Singlet-A
Excited State 1:	f=0.0000	<S**2>=2.000	495.24nm	2.5035eV	Triplet-A
Excited State 2:	f=0.0000	<S**2>=2.000	460.93nm	2.6899eV	Triplet-A
Excited State 3:	f=0.0000	<S**2>=2.000	433.79nm	2.8581eV	Triplet-A
Excited State 4:	f=0.0000	<S**2>=2.000	416.50nm	2.9768eV	Triplet-A
Excited State 5:	f=0.0000	<S**2>=2.000	396.82nm	3.1244eV	Triplet-A
Excited State 6:	f=0.0000	<S**2>=2.000	382.41nm	3.2422eV	Triplet-A
Excited State 7:	f=0.0000	<S**2>=2.000	374.65nm	3.3093eV	Triplet-A
Excited State 8:	f=0.0000	<S**2>=2.000	373.15nm	3.3227eV	Triplet-A
Excited State 9:	f=0.0000	<S**2>=2.000	363.36nm	3.4122eV	Triplet-A
Excited State 10:	f=0.0000	<S**2>=2.000	359.57nm	3.4481eV	Triplet-A

Pt-H-2

Excited State 1:	f=0.0121	<S**2>=0.000	368.27nm	3.3667eV	Singlet-A
Excited State 2:	f=0.0069	<S**2>=0.000	347.06nm	3.5724eV	Singlet-A
Excited State 3:	f=0.0301	<S**2>=0.000	334.71nm	3.7043eV	Singlet-A
Excited State 4:	f=0.0073	<S**2>=0.000	322.68nm	3.8423eV	Singlet-A
Excited State 5:	f=0.0046	<S**2>=0.000	317.21nm	3.9086eV	Singlet-A
Excited State 6:	f=0.0018	<S**2>=0.000	315.91nm	3.9247eV	Singlet-A
Excited State 7:	f=0.0704	<S**2>=0.000	309.38nm	4.0075eV	Singlet-A
Excited State 8:	f=0.0042	<S**2>=0.000	306.14nm	4.0500eV	Singlet-A
Excited State 9:	f=0.0063	<S**2>=0.000	304.89nm	4.0665eV	Singlet-A
Excited State 10:	f=0.0112	<S**2>=0.000	298.37nm	4.1554eV	Singlet-A
Excited State 1:	f=0.0000	<S**2>=2.000	443.12nm	2.7980eV	Triplet-A
Excited State 2:	f=0.0000	<S**2>=2.000	435.46nm	2.8472eV	Triplet-A
Excited State 3:	f=0.0000	<S**2>=2.000	432.81nm	2.8646eV	Triplet-A
Excited State 4:	f=0.0000	<S**2>=2.000	376.30nm	3.2948eV	Triplet-A
Excited State 5:	f=0.0000	<S**2>=2.000	365.40nm	3.3931eV	Triplet-A
Excited State 6:	f=0.0000	<S**2>=2.000	353.82nm	3.5042eV	Triplet-A
Excited State 7:	f=0.0000	<S**2>=2.000	344.36nm	3.6004eV	Triplet-A
Excited State 8:	f=0.0000	<S**2>=2.000	343.66nm	3.6078eV	Triplet-A

Excited State 9:	f=0.0000	<S**2>=2.000	332.77nm	3.7259eV	Triplet-A
Excited State 10:	f=0.0000	<S**2>=2.000	331.50nm	3.7401eV	Triplet-A

Pt-CHO

Excited State 1:	f=0.0090	<S**2>=0.000	431.70nm	2.8720eV	Singlet-A
Excited State 2:	f=0.0518	<S**2>=0.000	400.69nm	3.0943eV	Singlet-A
Excited State 3:	f=0.0161	<S**2>=0.000	394.65nm	3.1416eV	Singlet-A
Excited State 4:	f=0.0386	<S**2>=0.000	379.27nm	3.2690eV	Singlet-A
Excited State 5:	f=0.0032	<S**2>=0.000	367.39nm	3.3747eV	Singlet-A
Excited State 6:	f=0.0021	<S**2>=0.000	355.81nm	3.4846eV	Singlet-A
Excited State 7:	f=0.0175	<S**2>=0.000	353.75nm	3.5049eV	Singlet-A
Excited State 8:	f=0.0058	<S**2>=0.000	351.36nm	3.5287eV	Singlet-A
Excited State 9:	f=0.0132	<S**2>=0.000	344.27nm	3.6013eV	Singlet-A
Excited State 10:	f=0.0598	<S**2>=0.000	332.94nm	3.7239eV	Singlet-A

Excited State 1:	f=0.0000	<S**2>=2.000	530.37nm	2.3377eV	Triplet-A
Excited State 2:	f=0.0000	<S**2>=2.000	504.86nm	2.4558eV	Triplet-A
Excited State 3:	f=0.0000	<S**2>=2.000	434.41nm	2.8541eV	Triplet-A
Excited State 4:	f=0.0000	<S**2>=2.000	434.17nm	2.8557eV	Triplet-A
Excited State 5:	f=0.0000	<S**2>=2.000	423.58nm	2.9271eV	Triplet-A
Excited State 6:	f=0.0000	<S**2>=2.000	419.22nm	2.9575eV	Triplet-A
Excited State 7:	f=0.0000	<S**2>=2.000	415.02nm	2.9875eV	Triplet-A
Excited State 8:	f=0.0000	<S**2>=2.000	407.66nm	3.0413eV	Triplet-A
Excited State 9:	f=0.0000	<S**2>=2.000	398.28nm	3.1130eV	Triplet-A
Excited State 10:	f=0.0000	<S**2>=2.000	392.84nm	3.1561eV	Triplet-A

Pt-CHO-2

Excited State 1:	f=0.0089	<S**2>=0.000	412.58nm	3.0051eV	Singlet-A
Excited State 2:	f=0.0046	<S**2>=0.000	386.58nm	3.2072eV	Singlet-A
Excited State 3:	f=0.0148	<S**2>=0.000	359.60nm	3.4478eV	Singlet-A
Excited State 4:	f=0.0277	<S**2>=0.000	356.91nm	3.4739eV	Singlet-A
Excited State 5:	f=0.0001	<S**2>=0.000	352.90nm	3.5133eV	Singlet-A
Excited State 6:	f=0.0083	<S**2>=0.000	349.74nm	3.5450eV	Singlet-A
Excited State 7:	f=0.0404	<S**2>=0.000	340.71nm	3.6390eV	Singlet-A
Excited State 8:	f=0.0059	<S**2>=0.000	338.14nm	3.6666eV	Singlet-A
Excited State 9:	f=0.0024	<S**2>=0.000	323.66nm	3.8306eV	Singlet-A
Excited State 10:	f=0.0085	<S**2>=0.000	319.94nm	3.8753eV	Singlet-A

Excited State 1:	f=0.0000	<S**2>=2.000	485.89nm	2.5517eV	Triplet-A
Excited State 2:	f=0.0000	<S**2>=2.000	479.78nm	2.5842eV	Triplet-A
Excited State 3:	f=0.0000	<S**2>=2.000	435.27nm	2.8484eV	Triplet-A
Excited State 4:	f=0.0000	<S**2>=2.000	419.79nm	2.9535eV	Triplet-A
Excited State 5:	f=0.0000	<S**2>=2.000	416.74nm	2.9751eV	Triplet-A
Excited State 6:	f=0.0000	<S**2>=2.000	412.88nm	3.0029eV	Triplet-A

Excited State 7:	f=0.0000	<S**2>=2.000	395.88nm	3.1319eV	Triplet-A
Excited State 8:	f=0.0000	<S**2>=2.000	372.51nm	3.3284eV	Triplet-A
Excited State 9:	f=0.0000	<S**2>=2.000	361.39nm	3.4308eV	Triplet-A
Excited State 10:	f=0.0000	<S**2>=2.000	360.04nm	3.4437eV	Triplet-A

Pt-COOH

Excited State 1:	f=0.0071	<S**2>=0.000	427.70nm	2.8989eV	Singlet-A
Excited State 2:	f=0.0627	<S**2>=0.000	395.81nm	3.1324eV	Singlet-A
Excited State 3:	f=0.0070	<S**2>=0.000	389.17nm	3.1859eV	Singlet-A
Excited State 4:	f=0.0487	<S**2>=0.000	372.28nm	3.3304eV	Singlet-A
Excited State 5:	f=0.0030	<S**2>=0.000	357.24nm	3.4706eV	Singlet-A
Excited State 6:	f=0.0230	<S**2>=0.000	348.04nm	3.5624eV	Singlet-A
Excited State 7:	f=0.0197	<S**2>=0.000	336.34nm	3.6862eV	Singlet-A
Excited State 8:	f=0.0433	<S**2>=0.000	333.50nm	3.7176eV	Singlet-A
Excited State 9:	f=0.0021	<S**2>=0.000	327.36nm	3.7874eV	Singlet-A
Excited State 10:	f=0.0002	<S**2>=0.000	319.08nm	3.8856eV	Singlet-A

Excited State 1:	f=0.0000	<S**2>=2.000	517.73nm	2.3948eV	Triplet-A
Excited State 2:	f=0.0000	<S**2>=2.000	488.91nm	2.5359eV	Triplet-A
Excited State 3:	f=0.0000	<S**2>=2.000	434.23nm	2.8553eV	Triplet-A
Excited State 4:	f=0.0000	<S**2>=2.000	427.58nm	2.8997eV	Triplet-A
Excited State 5:	f=0.0000	<S**2>=2.000	411.92nm	3.0099eV	Triplet-A
Excited State 6:	f=0.0000	<S**2>=2.000	402.17nm	3.0828eV	Triplet-A
Excited State 7:	f=0.0000	<S**2>=2.000	390.37nm	3.1760eV	Triplet-A
Excited State 8:	f=0.0000	<S**2>=2.000	387.49nm	3.1997eV	Triplet-A
Excited State 9:	f=0.0000	<S**2>=2.000	365.57nm	3.3916eV	Triplet-A
Excited State 10:	f=0.0000	<S**2>=2.000	362.04nm	3.4246eV	Triplet-A

Pt-COOH-2

Excited State 1:	f=0.0102	<S**2>=0.000	401.30nm	3.0896eV	Singlet-A
Excited State 2:	f=0.0046	<S**2>=0.000	376.88nm	3.2898eV	Singlet-A
Excited State 3:	f=0.0454	<S**2>=0.000	347.83nm	3.5645eV	Singlet-A
Excited State 4:	f=0.0047	<S**2>=0.000	346.26nm	3.5807eV	Singlet-A
Excited State 5:	f=0.0039	<S**2>=0.000	330.57nm	3.7507eV	Singlet-A
Excited State 6:	f=0.0512	<S**2>=0.000	329.61nm	3.7615eV	Singlet-A
Excited State 7:	f=0.0044	<S**2>=0.000	324.13nm	3.8251eV	Singlet-A
Excited State 8:	f=0.0003	<S**2>=0.000	314.11nm	3.9471eV	Singlet-A
Excited State 9:	f=0.0156	<S**2>=0.000	312.03nm	3.9735eV	Singlet-A
Excited State 10:	f=0.0495	<S**2>=0.000	309.23nm	4.0094eV	Singlet-A

Excited State 1:	f=0.0000	<S**2>=2.000	467.82nm	2.6503eV	Triplet-A
Excited State 2:	f=0.0000	<S**2>=2.000	460.21nm	2.6941eV	Triplet-A
Excited State 3:	f=0.0000	<S**2>=2.000	435.09nm	2.8496eV	Triplet-A
Excited State 4:	f=0.0000	<S**2>=2.000	407.80nm	3.0403eV	Triplet-A

Excited State 5:	f=0.0000	<S**2>=2.000	387.76nm	3.1974eV	Triplet-A
Excited State 6:	f=0.0000	<S**2>=2.000	366.00nm	3.3876eV	Triplet-A
Excited State 7:	f=0.0000	<S**2>=2.000	354.75nm	3.4949eV	Triplet-A
Excited State 8:	f=0.0000	<S**2>=2.000	350.01nm	3.5423eV	Triplet-A
Excited State 9:	f=0.0000	<S**2>=2.000	348.85nm	3.5541eV	Triplet-A
Excited State 10:	f=0.0000	<S**2>=2.000	346.36nm	3.5796eV	Triplet-A