A Trojan Horse Approach to Enhancing the Cell Income of a Ruthenium Nitrosyl Complex

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S1. DFT Computations

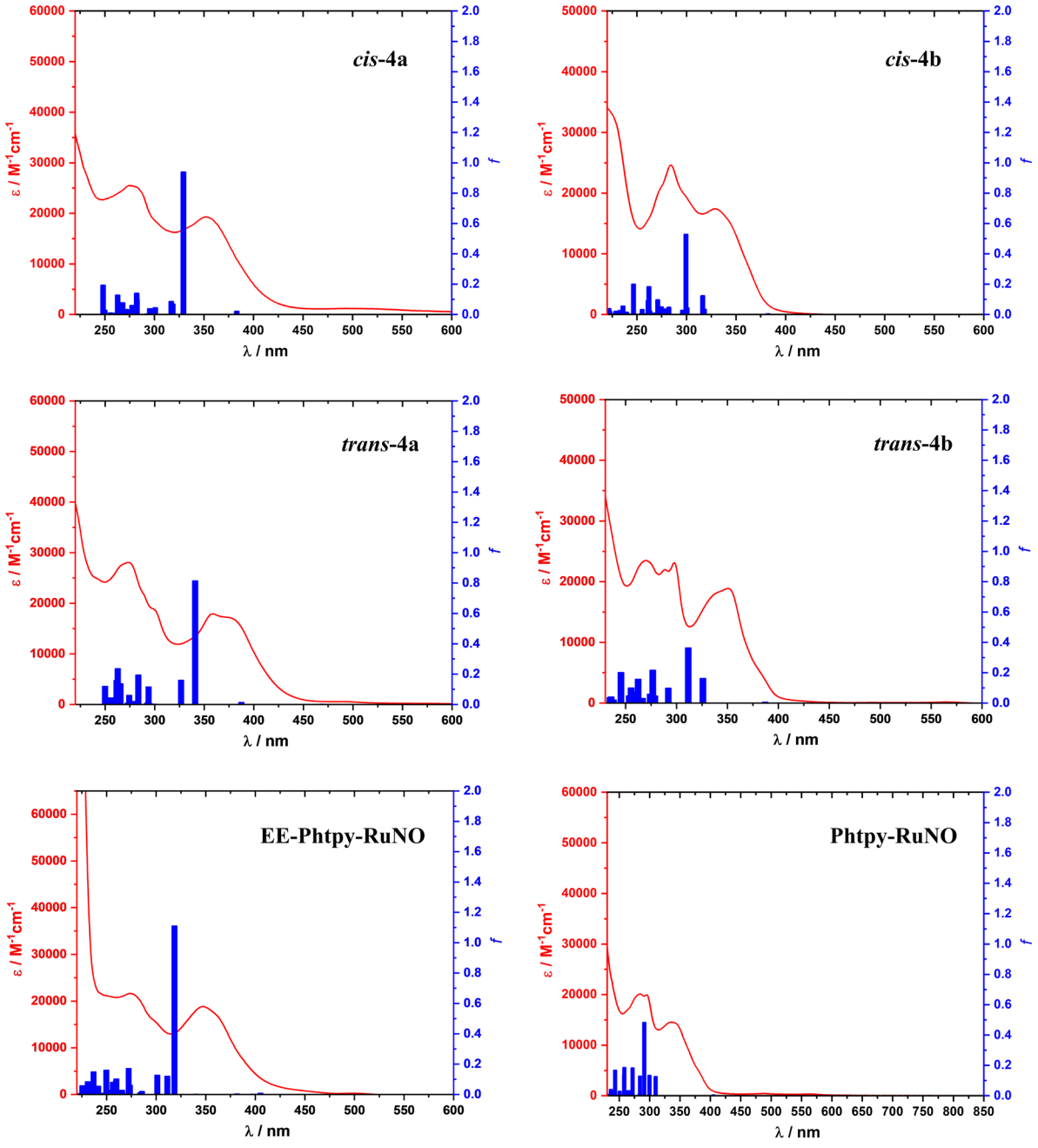


Figure S1. Comparison among the experimental UV-Vis spectra and the TD-DFT (CAM-B3LYP/6-31G*) computed excitations for complexes ***cis*-4a-b**/***trans*-4a-b** in acetonitrile and **EE-Phtpy-RuNO**/**Phtpy-RuNO** in water (+0.5 % DMSO for the experimental spectra).

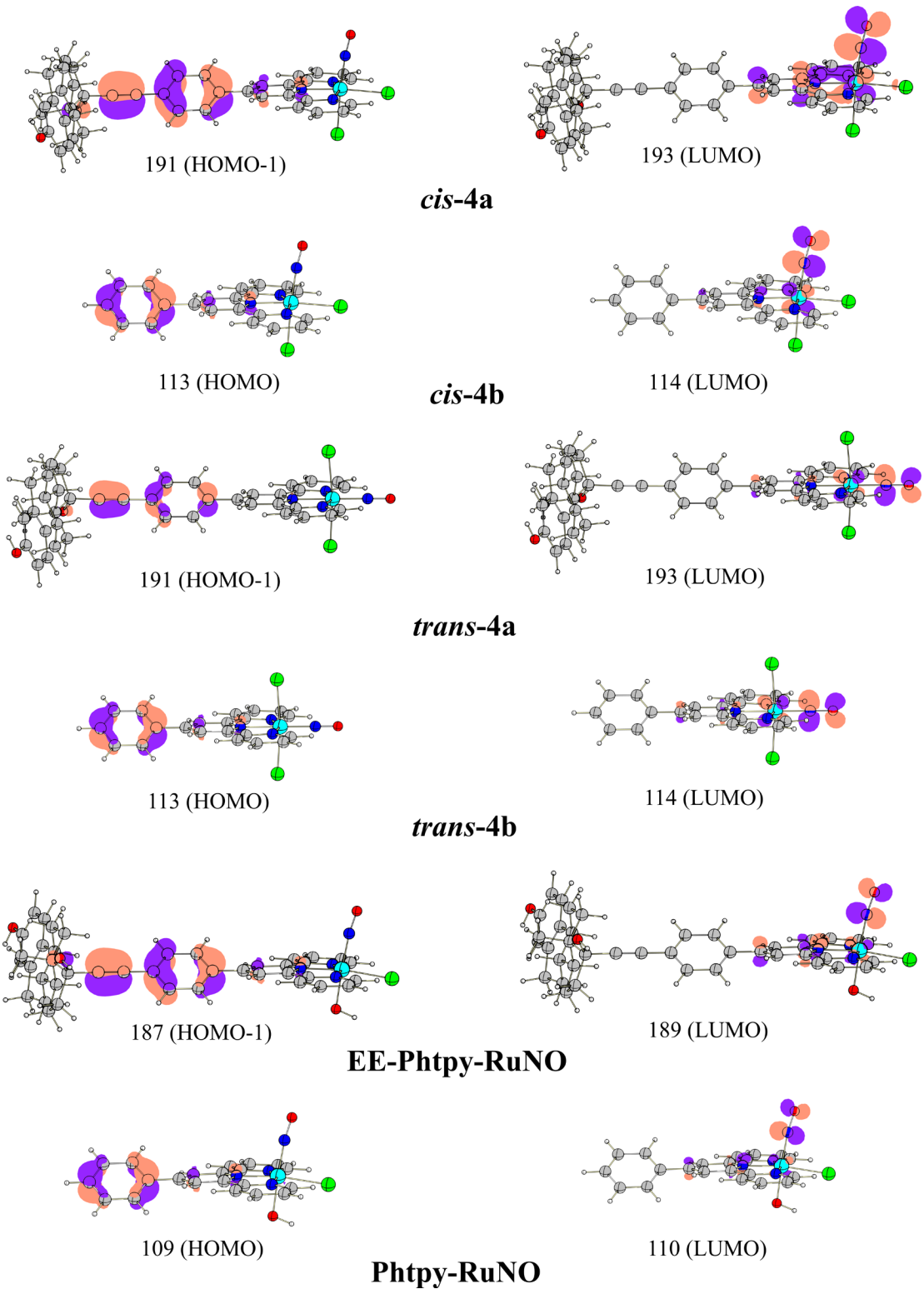


Figure S2. Relevant molecular orbitals for the investigated RuNO complexes computed by TD-DFT at the CAM-B3LYP/6-31G* level of theory.

Optimized coordinates

[*cis*-4a]$^+$

O	5.98810	-4.42300	-1.26820
H	5.34230	-5.10140	-1.01630
O	10.89480	5.31430	-0.23240
H	11.34820	5.40900	0.61930
C	6.36230	-3.87300	1.13800
H	6.99520	-4.75690	1.00760
H	5.49520	-4.17940	1.73070
C	10.14060	4.17830	-0.21270
C	4.55320	-2.86460	-0.23750
C	3.39130	-2.50790	-0.19540
C	8.30250	-2.97270	-0.98120
H	9.10690	-2.24430	-1.11380
H	8.18590	-3.51750	-1.92250
H	8.63280	-3.69050	-0.22410
C	6.97800	-2.28300	-0.60990
C	5.92860	-3.39320	-0.28640
C	6.59740	-1.26980	-1.69450
H	5.57180	-0.92050	-1.51420
H	6.60250	-1.74090	-2.68620
C	7.54010	-0.05550	-1.69250
H	8.54330	-0.34180	-2.03540
H	7.16190	0.66210	-2.42950
C	7.64560	0.61110	-0.30740
H	6.62580	0.94850	-0.04690
C	8.54690	1.84170	-0.27450
C	8.62620	2.71320	-1.37230
H	8.05910	2.49710	-2.27310
C	10.07040	3.33440	0.89400
H	10.63580	3.57900	1.79330
C	9.40610	3.86340	-1.35850
H	9.45150	4.52110	-2.22210
C	9.28390	2.17580	0.87780
C	9.27190	1.30500	2.11630
H	9.23620	1.94070	3.01040
H	10.22870	0.76400	2.17400
C	7.14070	-2.69790	1.78220
H	6.72480	-2.41400	2.75390
H	8.18860	-2.97300	1.95200
C	7.03030	-1.56090	0.75390
H	6.03550	-1.10390	0.89110
C	8.03680	-0.41430	0.78050
H	9.03810	-0.80900	0.54510
C	8.13000	0.29220	2.13200
H	7.17590	0.79680	2.34480
H	8.29340	-0.43090	2.94010
Ru	-6.55720	0.64380	0.13510
Cl	-6.42010	0.60690	-2.22900
N	-4.66660	0.04520	0.10940
C	-4.42380	-1.27700	0.06280
C	-5.64480	-2.10880	0.02620
N	-5.58520	2.49310	0.04910
C	-0.65420	-1.22570	-0.04860

N	-6.82710	-1.42640	0.03210
C	-8.03860	-3.47310	-0.08810
H	-8.99990	-3.97230	-0.13360
C	-3.70700	0.98660	0.06660
C	-2.37700	0.58870	0.02230
H	-1.58510	1.32740	0.02150
C	-5.39880	4.86520	-0.04550
H	-5.89750	5.82700	-0.08330
C	-4.22560	2.37060	0.04680
C	-2.05850	-0.78120	0.00170
C	-5.63540	-3.49750	-0.03270
H	-4.69740	-4.04000	-0.03600
C	-3.10780	-1.71820	0.01310
H	-2.88860	-2.77680	-0.05320
C	-7.98880	-2.08350	-0.02490
H	-8.88160	-1.46810	-0.02000
C	-6.15740	3.69920	0.00090
H	-7.24190	3.70860	-0.00130
C	-3.41890	3.50210	0.00370
H	-2.33940	3.40740	0.00220
C	-4.01270	4.76240	-0.04120
H	-3.39180	5.65160	-0.07450
C	-6.84570	-4.18650	-0.09010
H	-6.84920	-5.27050	-0.13680
Cl	-8.87930	1.38440	-0.07200
C	-0.25100	-2.40270	0.60390
H	-0.96820	-2.98140	1.17900
C	1.62930	-0.90170	-0.80640
H	2.35850	-0.32550	-1.36710
C	1.07130	-2.81990	0.56290
C	0.30850	-0.48190	-0.75160
H	0.01870	0.41440	-1.29230
C	2.03420	-2.07720	-0.14620
N	-6.79670	0.71040	1.87330
O	-7.06200	0.78560	2.97990
H	1.37150	-3.72290	1.08520

[*cis*-4b]$^{+}$

H	8.27740	-0.00220	0.03720
Ru	-1.80830	-0.00330	0.10160
Cl	-1.66230	0.06040	-2.26160
N	0.17420	-0.00150	0.08830
C	0.80640	-1.18710	0.02910
C	-0.10510	-2.34820	-0.04680
N	-1.44100	2.05490	0.06380
C	4.38720	0.00130	0.03890
N	-1.43860	-2.05540	-0.04960
C	-1.97330	-4.36820	-0.23590
H	-2.73790	-5.13310	-0.31060
C	0.80480	1.18620	0.08540
C	2.19380	1.21030	0.07190
H	2.72480	2.15390	0.10410
C	-1.97810	4.37400	0.00670
H	-2.74360	5.14100	-0.02330
C	-0.10780	2.34860	0.07820

C	2.91190	0.00150	0.04360
C	0.32420	-3.66740	-0.13350
H	1.38230	-3.90050	-0.13110
C	2.19520	-1.20830	0.00950
H	2.72720	-2.14910	-0.06300
C	-2.34670	-3.03060	-0.14340
H	-3.38370	-2.71350	-0.14350
C	-2.35010	3.03300	0.02700
H	-3.38710	2.71570	0.01290
C	0.32020	3.67090	0.06180
H	1.37820	3.90450	0.07250
C	-0.62560	4.69420	0.02640
H	-0.30180	5.72980	0.01280
C	-0.62060	-4.68790	-0.22840
H	-0.29570	-5.72090	-0.29730
Cl	-4.24470	0.00280	-0.10990
C	5.09940	-1.00400	0.71320
H	4.56560	-1.77170	1.26660
C	6.49190	0.99880	-0.63960
H	7.03090	1.77370	-1.17730
C	6.49100	-1.00050	0.71570
C	5.10030	1.00530	-0.63610
H	4.56830	1.77420	-1.18950
C	7.19100	-0.00130	0.03780
N	-2.06200	-0.05270	1.83810
O	-2.34220	-0.08680	2.94300
H	7.02890	-1.77640	1.25300

[*trans*-4a]$^{+}$

O	5.95660	-4.48010	-1.07340
H	5.30390	-5.14240	-0.79740
O	10.95910	5.23490	-0.46550
H	11.39590	5.37110	0.38930
C	6.29410	-3.81000	1.30770
H	6.92570	-4.70120	1.23260
H	5.41590	-4.08340	1.90000
C	10.18410	4.11500	-0.39690
C	4.51360	-2.86520	-0.14600
C	3.35270	-2.50260	-0.13670
C	8.27450	-3.02690	-0.82110
H	9.08160	-2.30910	-0.99010
H	8.16740	-3.62990	-1.72730
H	8.59460	-3.69520	-0.01590
C	6.94730	-2.31370	-0.50860
C	5.88680	-3.40140	-0.14650
C	6.58960	-1.35510	-1.64900
H	5.56260	-0.99340	-1.50360
H	6.60880	-1.87530	-2.61570
C	7.53840	-0.14620	-1.69300
H	8.54390	-0.45370	-2.00980
H	7.17290	0.53630	-2.46850
C	7.63190	0.58830	-0.34200
H	6.61290	0.95120	-0.11460
C	8.55020	1.80630	-0.35940
C	8.66870	2.61080	-1.50380

H	8.11840	2.35170	-2.40360
C	10.07510	3.33830	0.75510
H	10.62590	3.62530	1.65090
C	9.46900	3.74640	-1.53890
H	9.54560	4.35150	-2.43800
C	9.26870	2.19380	0.78800
C	9.21810	1.39380	2.07280
H	9.16750	2.07910	2.92880
H	10.16850	0.84960	2.18330
C	7.06610	-2.60630	1.90470
H	6.63360	-2.27070	2.85230
H	8.10920	-2.87670	2.10830
C	6.98050	-1.52330	0.81710
H	5.98660	-1.05420	0.91350
C	7.99440	-0.38340	0.80400
H	8.99700	-0.79640	0.60850
C	8.06720	0.39190	2.11850
H	7.11360	0.91420	2.28530
H	8.20840	-0.28870	2.96670
Ru	-6.62840	0.68330	0.03580
Cl	-6.49230	0.79390	-2.37110
Cl	-6.47170	0.47810	2.43450
N	-4.71660	0.07370	-0.01550
C	-4.46330	-1.24530	-0.09290
C	-5.67660	-2.07650	-0.14380
N	-5.60420	2.50270	0.15280
C	-0.69250	-1.21280	-0.08810
N	-6.85300	-1.39100	-0.09580
C	-8.06200	-3.44600	-0.21680
H	-9.02530	-3.94260	-0.24190
C	-3.74310	1.00100	0.03400
C	-2.41360	0.60260	0.01060
H	-1.62200	1.33780	0.08280
C	-5.39400	4.87580	0.30910
H	-5.88960	5.83720	0.38160
C	-4.24740	2.38070	0.12650
C	-2.09540	-0.76450	-0.06720
C	-5.66430	-3.46420	-0.23200
H	-4.72340	-3.99990	-0.27190
C	-3.14960	-1.69250	-0.12160
H	-2.93610	-2.75040	-0.21040
C	-8.01280	-2.05900	-0.13040
H	-8.92000	-1.47000	-0.08740
C	-6.16040	3.71720	0.24450
H	-7.24180	3.76230	0.26780
C	-3.43060	3.50460	0.18660
H	-2.35260	3.39820	0.16250
C	-4.00910	4.76770	0.27760
H	-3.38150	5.65140	0.32400
C	-6.87030	-4.15870	-0.26890
H	-6.87280	-5.24150	-0.33720
N	-8.30830	1.21800	0.06880
O	-9.39470	1.56160	0.08130
C	-0.31770	-2.42310	0.51950
H	-1.05730	-3.02690	1.03750
C	1.62000	-0.86000	-0.73780

H	2.37210	-0.25900	-1.23910
C	1.00410	-2.84280	0.50980
C	0.29900	-0.43820	-0.71380
H	0.03190	0.48560	-1.21880
C	1.99590	-2.06890	-0.12220
H	1.28190	-3.77150	0.99810

[*trans*-4b]$^{+}$

H	-8.22913	-0.00006	0.00023
Ru	1.89569	0.00002	0.00018
Cl	1.74239	0.07226	2.40720
Cl	1.74349	-0.07216	-2.40694
N	-0.11166	0.00002	-0.00023
C	-0.75594	-1.18053	0.02861
C	0.14570	-2.34314	0.06411
N	1.47571	2.04721	-0.05852
C	-4.33940	-0.00002	-0.00009
N	1.47574	-2.04718	0.05871
C	1.99973	-4.37546	0.12374
H	2.76564	-5.14233	0.14596
C	-0.75595	1.18056	-0.02908
C	-2.14401	1.20605	-0.03172
H	-2.67228	2.15000	-0.08464
C	1.99974	4.37548	-0.12375
H	2.76567	5.14234	-0.14580
C	0.14568	2.34318	-0.06449
C	-2.86479	0.00001	-0.00017
C	-0.28969	-3.66322	0.09931
H	-1.34962	-3.88754	0.10267
C	-2.14400	-1.20603	0.03129
H	-2.67228	-2.14997	0.08425
C	2.37649	-3.03746	0.08706
H	3.42089	-2.75249	0.07906
C	2.37649	3.03748	-0.08668
H	3.42087	2.75250	-0.07819
C	-0.28969	3.66324	-0.10015
H	-1.34962	3.88757	-0.10403
C	0.64686	4.69285	-0.13079
H	0.31857	5.72652	-0.15912
C	0.64684	-4.69284	0.13012
H	0.31854	-5.72651	0.15809
N	3.65883	-0.00009	0.00030
O	4.79831	-0.00025	0.00013
C	-5.05217	-1.01094	-0.66550
H	-4.51920	-1.78407	-1.21203
C	-6.44363	1.00596	0.66882
H	-6.98241	1.78584	1.19929
C	-6.44372	-1.00601	-0.66861
C	-5.05210	1.01088	0.66546
H	-4.51900	1.78397	1.21193
C	-7.14269	-0.00003	0.00014
H	-6.98260	-1.78591	-1.19897

[EE-Phtpy-RuNO]$^{+}$

O	-5.835644	-4.457676	1.098572
H	-5.180365	-5.117213	0.821918
O	-10.920286	5.211126	0.460963
H	-11.365495	5.337078	-0.391074
C	-6.198864	-3.808662	-1.284257
H	-6.824722	-4.702744	-1.196317
H	-5.324301	-4.082165	-1.881954
C	-10.135460	4.097986	0.393904
C	-4.411305	-2.840654	0.145845
C	-3.252071	-2.473311	0.125080
C	-8.165432	-3.021611	0.855200
H	-8.976208	-2.307858	1.024141
H	-8.047090	-3.615435	1.766106
H	-8.487417	-3.699416	0.058787
C	-6.845659	-2.302365	0.525583
C	-5.781021	-3.385531	0.162603
C	-6.484540	-1.332247	1.655309
H	-5.461508	-0.964623	1.497877
H	-6.491683	-1.844845	2.626245
C	-7.441446	-0.129759	1.698484
H	-8.441837	-0.442039	2.026603
H	-7.073949	0.561419	2.465300
C	-7.552474	0.593403	0.342687
H	-6.538498	0.962608	0.103617
C	-8.480728	1.803937	0.358933
C	-8.596517	2.615870	1.498391
H	-8.035933	2.368635	2.395204
C	-10.029188	3.313928	-0.753284
H	-10.590099	3.589525	-1.646349
C	-9.407073	3.744353	1.532314
H	-9.481089	4.355338	2.427664
C	-9.212477	2.176694	-0.785037
C	-9.165508	1.368291	-2.064646
H	-9.126744	2.048056	-2.925575
H	-10.112427	0.816076	-2.164285
C	-6.982859	-2.614360	-1.884351
H	-6.559783	-2.283351	-2.837795
H	-8.025841	-2.892657	-2.077835
C	-6.895624	-1.522427	-0.805843
H	-5.905960	-1.047035	-0.913996
C	-7.917497	-0.389696	-0.792718
H	-8.915353	-0.808274	-0.585369
C	-8.007146	0.375095	-2.112306
H	-7.059039	0.903540	-2.290885
H	-8.149913	-0.313037	-2.954154
Ru	6.701942	0.667362	-0.046133
N	4.813598	0.079069	0.059662
C	4.567120	-1.242253	0.088471
C	5.783029	-2.083962	0.094497
N	5.727631	2.520104	-0.213376
C	0.795427	-1.189424	0.054553
N	6.968795	-1.414373	0.023773
C	8.161993	-3.476544	0.057613
H	9.118267	-3.987054	0.039356

C	3.854254	1.016541	-0.034387
C	2.522419	0.620153	-0.038099
H	1.732000	1.354035	-0.136602
C	5.528601	4.883155	-0.444841
H	6.021961	5.842238	-0.555258
C	4.370337	2.396471	-0.165561
C	2.202050	-0.746923	0.040160
C	5.760357	-3.473272	0.151816
H	4.818302	-4.005421	0.211598
C	3.249482	-1.683185	0.090706
H	3.027506	-2.741667	0.148279
C	8.122697	-2.085890	0.005409
H	9.021169	-1.481550	-0.056307
C	6.291624	3.722611	-0.349445
H	7.375612	3.735693	-0.383849
C	3.557161	3.521407	-0.252269
H	2.478621	3.424964	-0.210089
C	4.143552	4.777998	-0.393138
H	3.518275	5.662243	-0.460998
C	6.963458	-4.176541	0.132838
H	6.957264	-5.260756	0.176898
Cl	8.991043	1.355420	-0.550590
C	0.411565	-2.387972	-0.569550
H	1.145123	-2.986303	-1.102213
C	-1.510889	-0.839254	0.728105
H	-2.256753	-0.243313	1.244606
C	-0.911532	-2.804374	-0.554052
C	-0.188325	-0.421160	0.699063
H	0.086652	0.494658	1.214530
C	-1.895366	-2.038509	0.099547
H	-1.196009	-3.725290	-1.053330
O	6.426388	0.466175	-1.948767
H	7.268748	0.705751	-2.371984
N	7.040675	0.877795	1.682684
O	7.401248	1.055111	2.757756

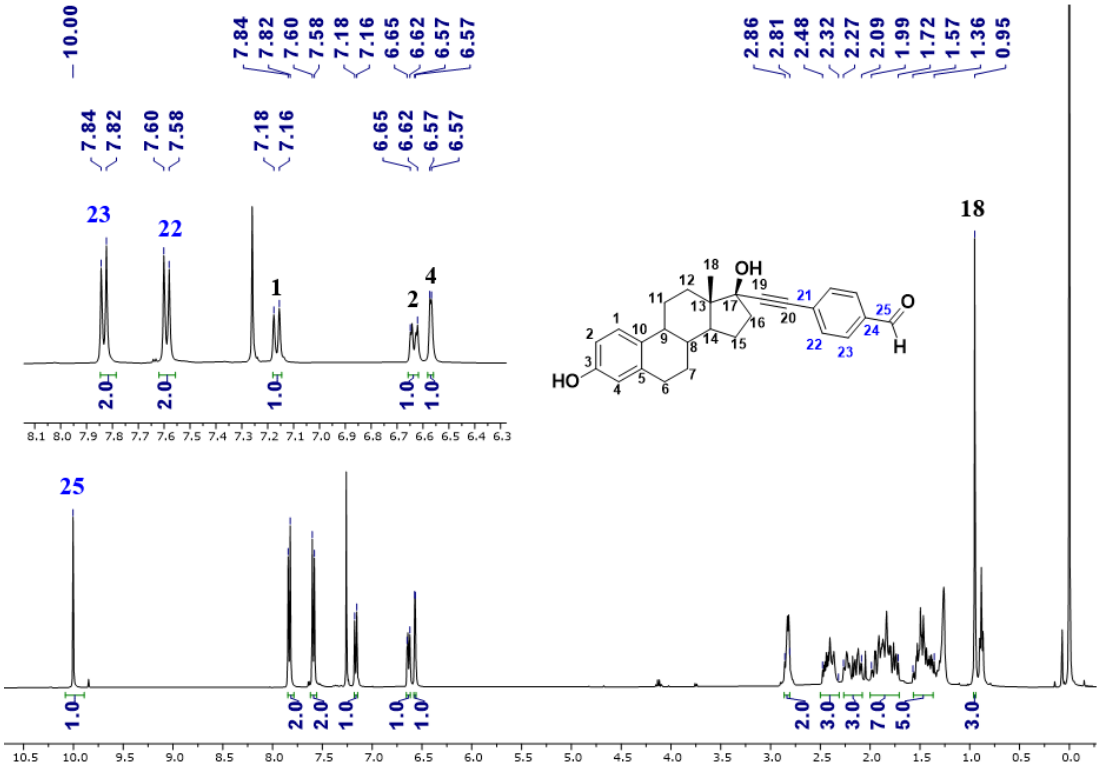
[Phtpy-RuNO]$^{+}$

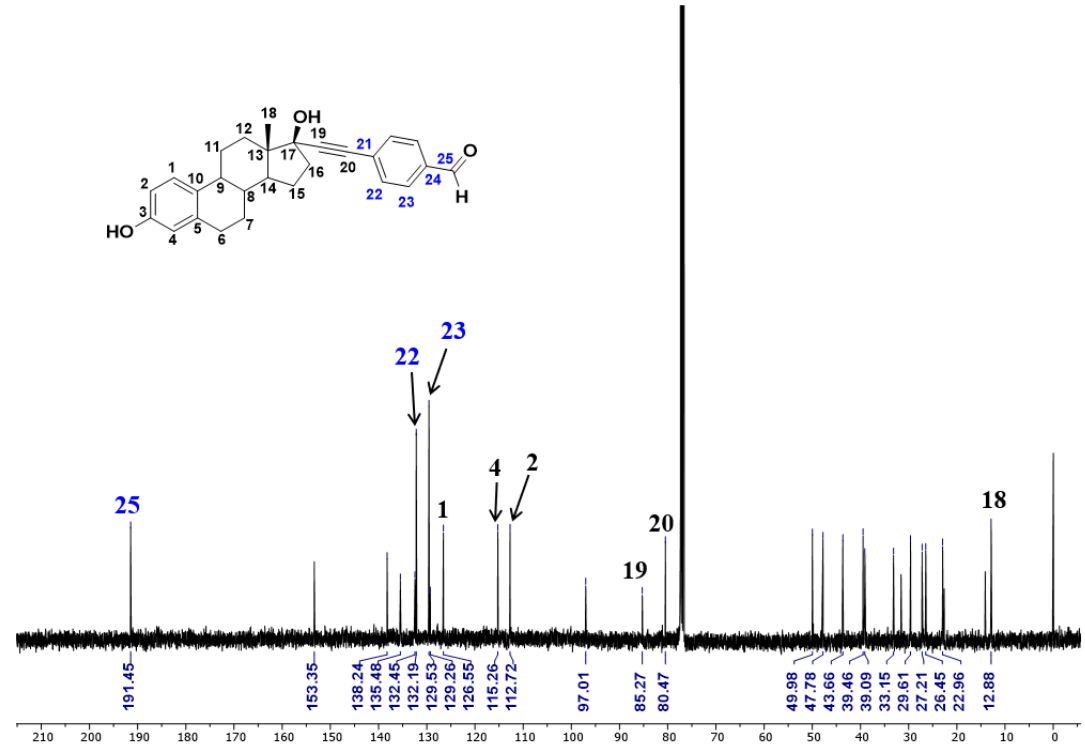
Ru	-1.85938	-0.00067	-0.02079
N	0.11901	0.00011	0.06254
C	0.74981	1.18724	0.05000
C	-0.15927	2.35375	0.02687
N	-1.48600	-2.06418	-0.12777
C	4.33441	0.00443	0.01402
H	8.22500	-0.00276	0.01431
N	-1.49166	2.06685	-0.02252
C	-2.01536	4.39068	-0.06228
H	-2.77588	5.16248	-0.09967
C	0.75299	-1.18386	-0.00187
C	2.14229	-1.20471	-0.01873
H	2.67533	-2.14469	-0.09458
C	-2.00355	-4.38394	-0.29039
H	-2.76185	-5.15465	-0.37061
C	-0.15299	-2.34983	-0.08924
C	2.85824	0.00490	0.01715

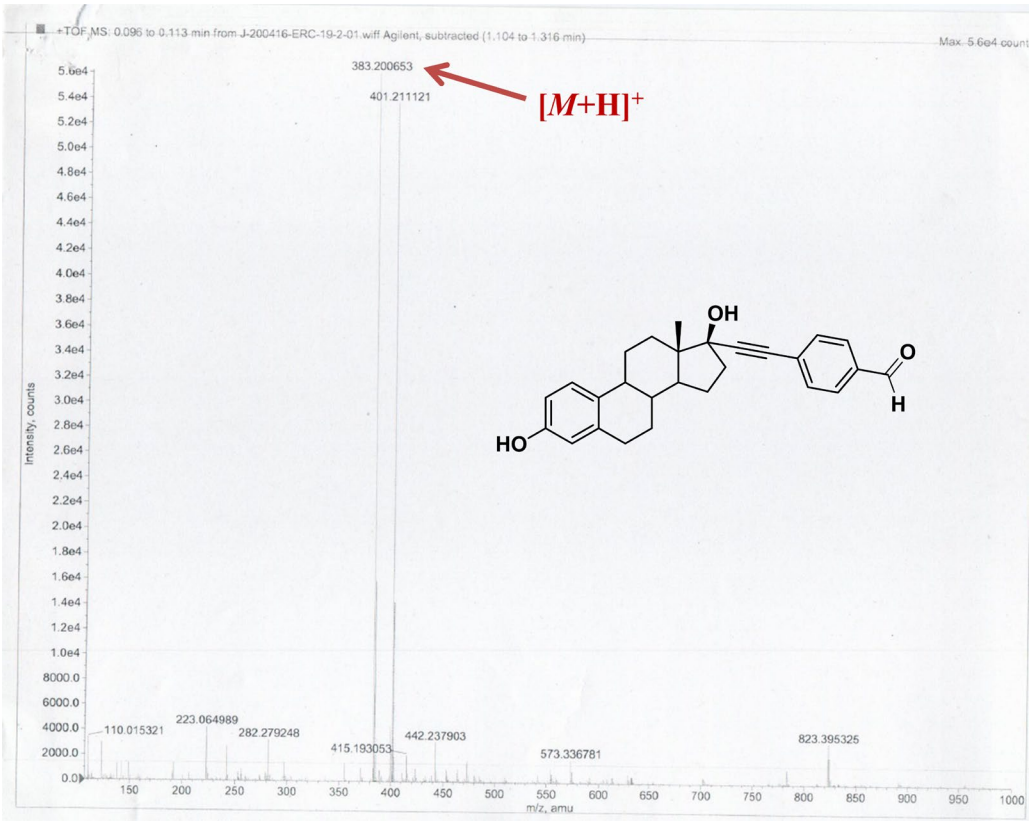
C	0.27699	3.67412	0.03603
H	1.33547	3.90229	0.07746
C	2.13932	1.21269	0.03965
H	2.66993	2.15670	0.06510
C	-2.39302	3.05077	-0.06637
H	-3.43118	2.73964	-0.10883
C	-2.38471	-3.04660	-0.22556
H	-3.42357	-2.73620	-0.25479
C	0.28664	-3.66793	-0.14661
H	1.34556	-3.89537	-0.11281
C	-0.64947	-4.69555	-0.24854
H	-0.31725	-5.72757	-0.29448
C	-0.66190	4.70326	-0.00883
H	-0.33235	5.73714	-0.00189
Cl	-4.25484	0.00756	-0.49947
C	5.04911	1.00316	-0.66693
H	4.51777	1.76905	-1.22509
C	6.43741	-0.99515	0.69773
H	6.97440	-1.76847	1.23965
C	6.44095	0.99600	-0.66951
C	5.04554	-0.99698	0.69476
H	4.51041	-1.76109	1.25193
C	7.13854	-0.00081	0.01424
H	6.98092	1.76711	-1.21165
O	-1.56115	0.04715	-1.93020
H	-2.44315	0.05037	-2.34031
N	-2.22669	-0.04569	1.71420
O	-2.61371	-0.07545	2.79435

S2. NMR and HRMS Spectra

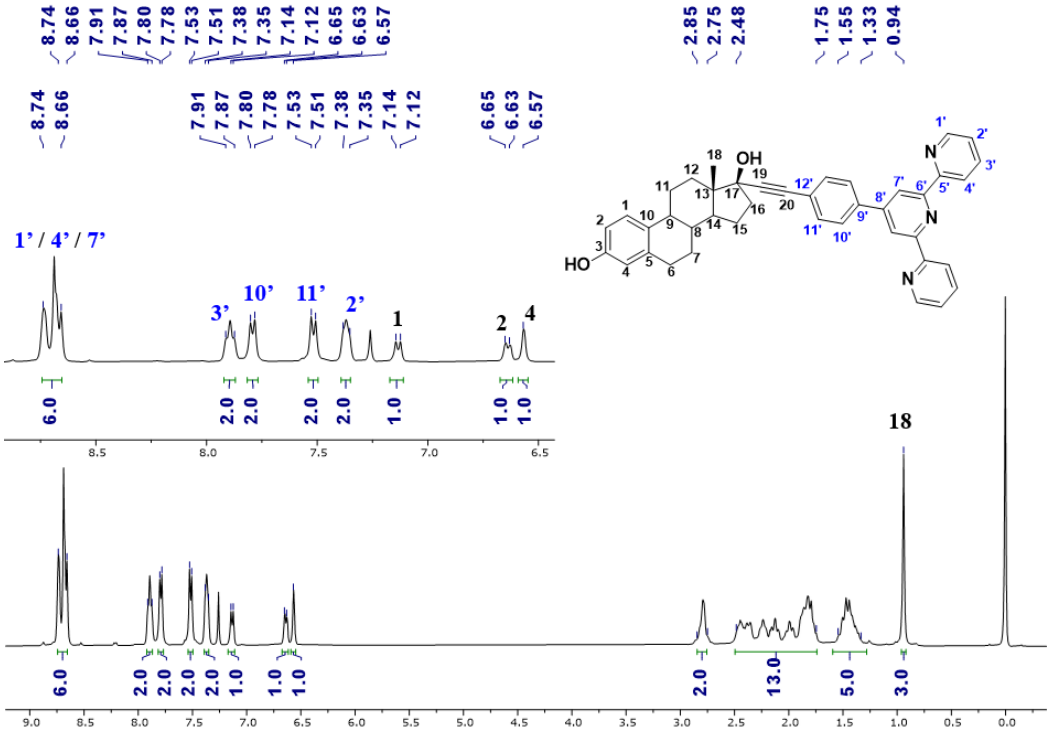
4-[3,17β-dihydroxy-19-norpregna-1,3,5(10)-trien-20-yn-21-yl]*benzaldehyde* (1a)

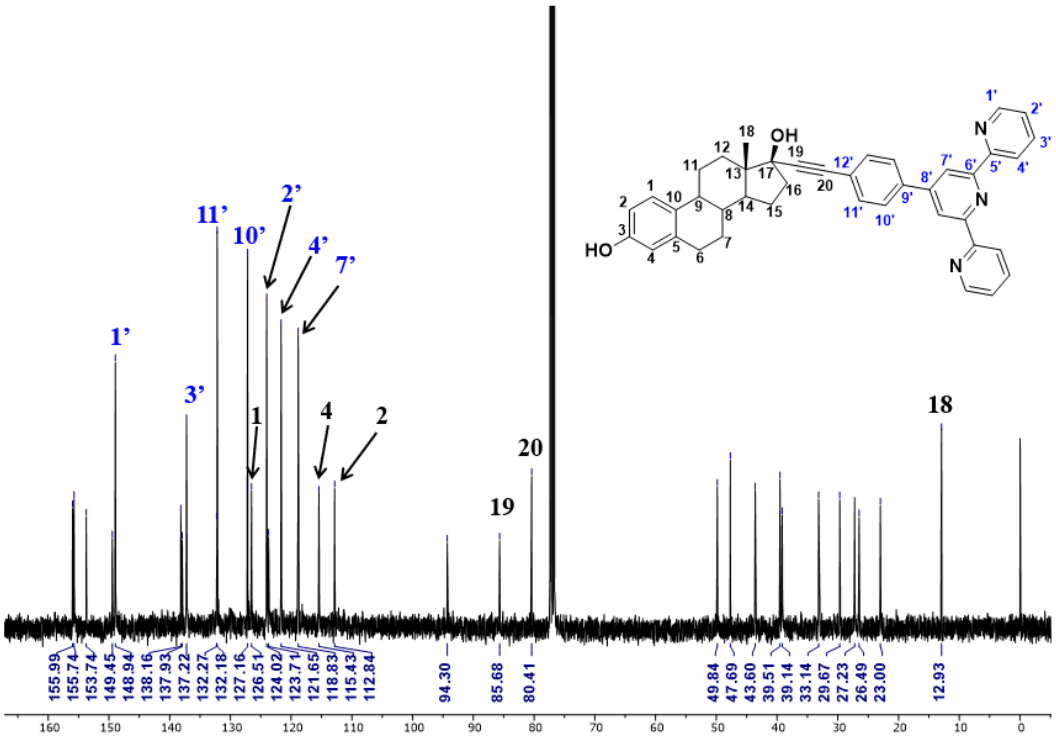


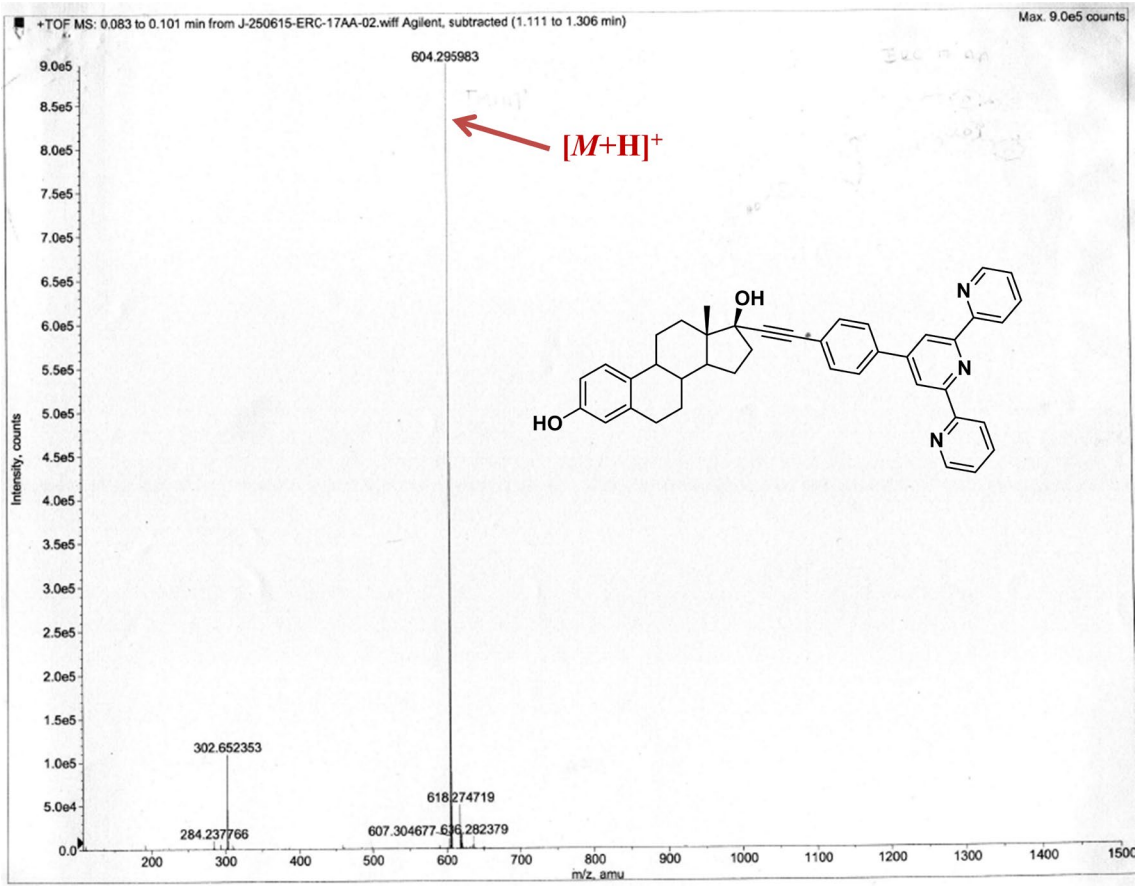




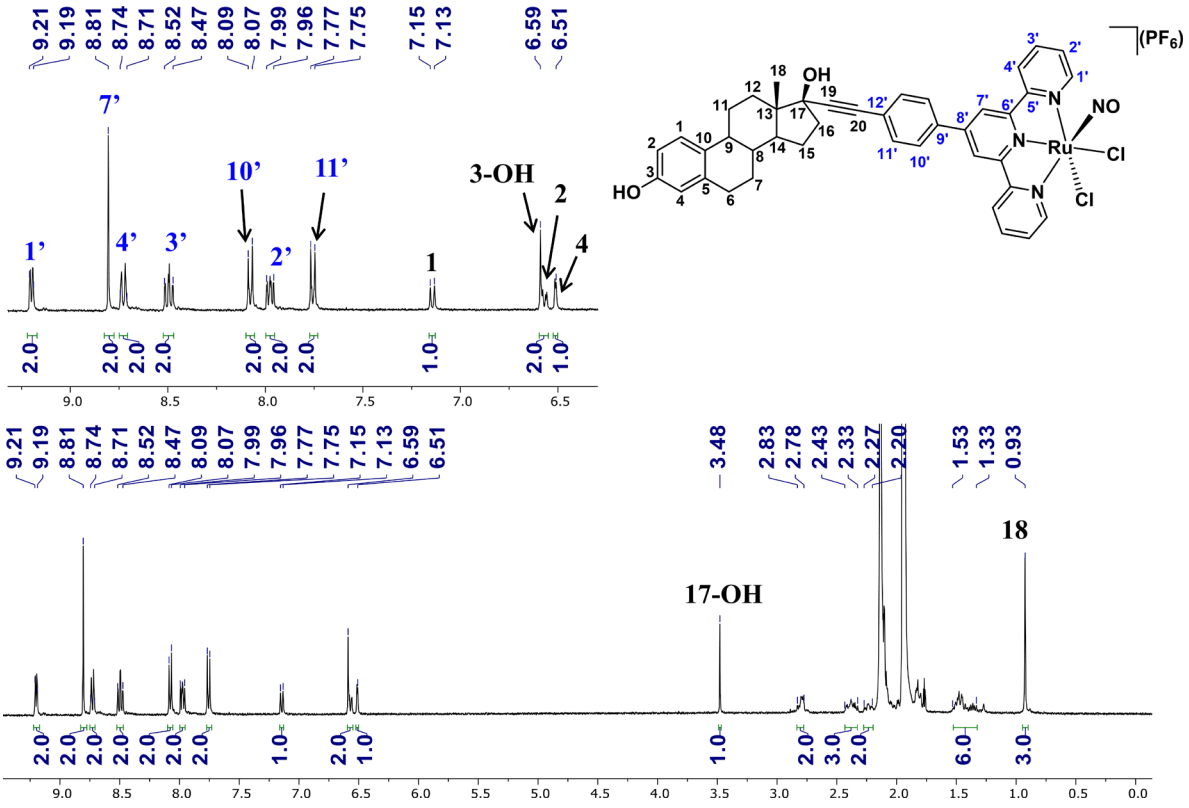
4'-(4-[3,17β-dihydroxy-19-norpregna-1,3,5(10)-trien-20-yn-21-yl]phenyl)-2,2':6',2''-terpyridine (2a, EE-Phtpy)

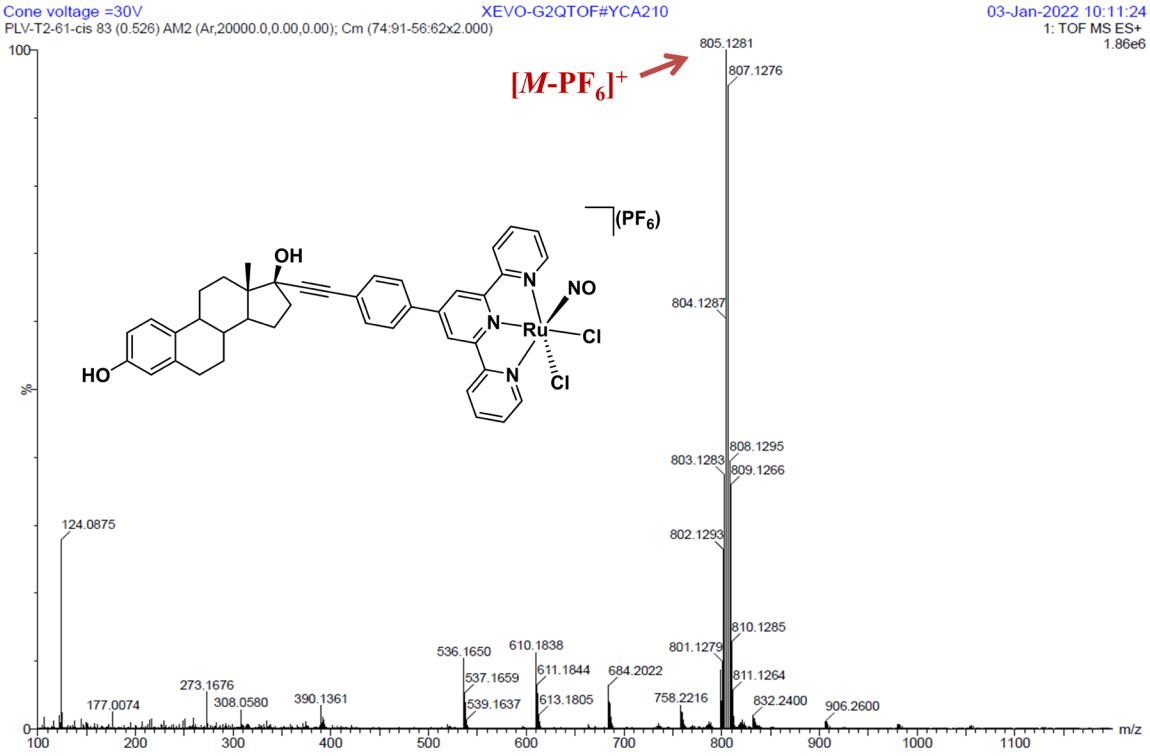



1'
2'
11'
10'
4'
7'
3'
1
4
2
20
19
18
155.99
155.74
153.74
149.45
148.94
138.16
137.93
137.22
132.27
132.18
127.16
126.51
124.02
123.71
121.65
118.83
115.43
112.84
94.30
85.68
80.41
49.84
47.69
43.60
39.51
39.14
33.14
29.67
27.23
26.49
23.00
12.93
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
OH
HO
N

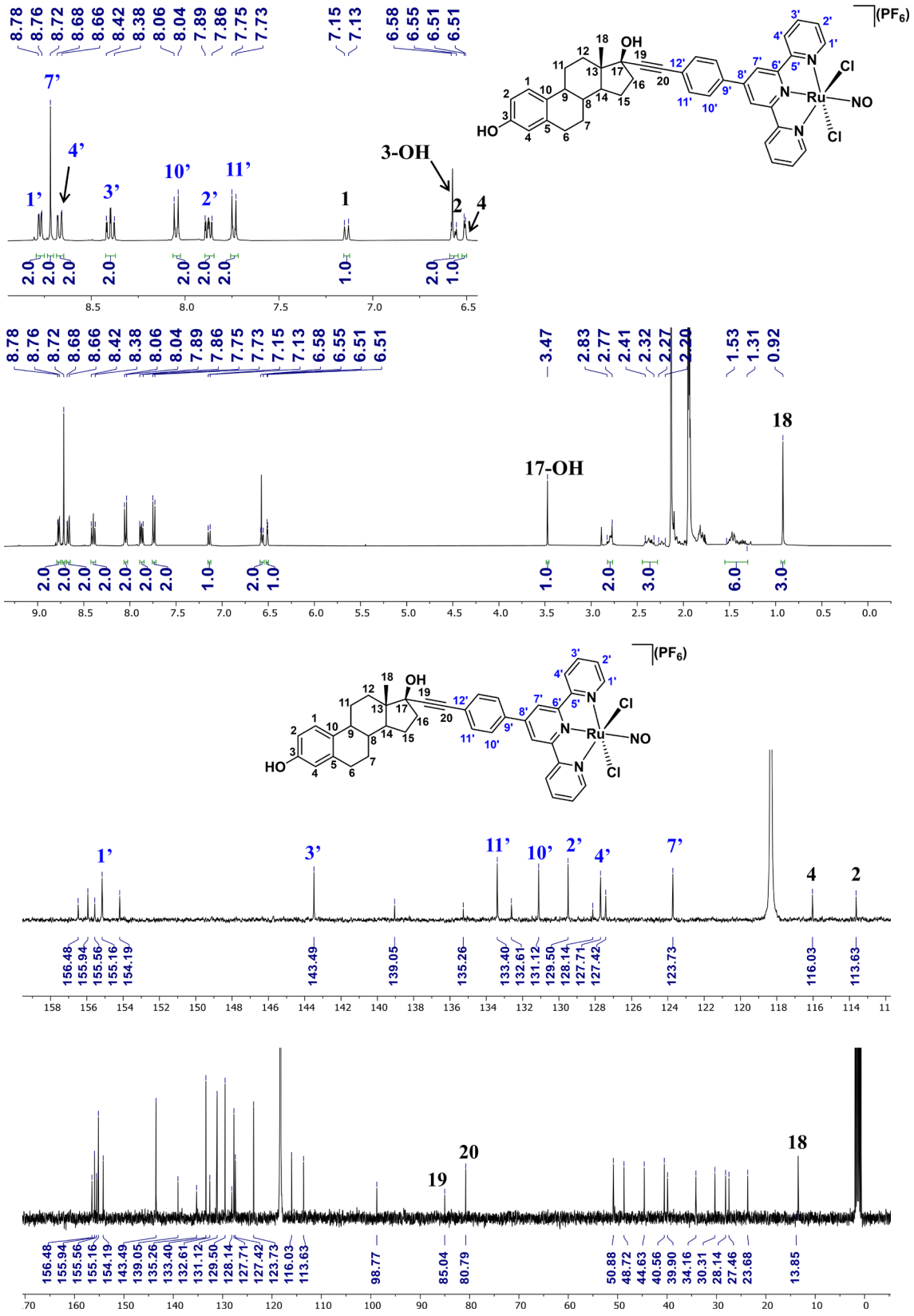

+TOF MS: 0.083 to 0.101 min from J-250615-ERC-17AA-02.wiff Agilent, subtracted (1.111 to 1.306 min)
Max. 9.0e5 counts.
604.295983
[M+H]+
Intensity, counts
9.0e5
8.5e5
8.0e5
7.5e5
7.0e5
6.5e5
6.0e5
5.5e5
5.0e5
4.5e5
4.0e5
3.5e5
3.0e5
2.5e5
2.0e5
1.5e5
1.0e5
5.0e4
0.0
302.652353
284.237766
618.274719
607.304677
636.282379
200
300
400
500
600
700
800
900
1000
1100
1200
1300
1400
1500
m/z, amu
OH
HO
N

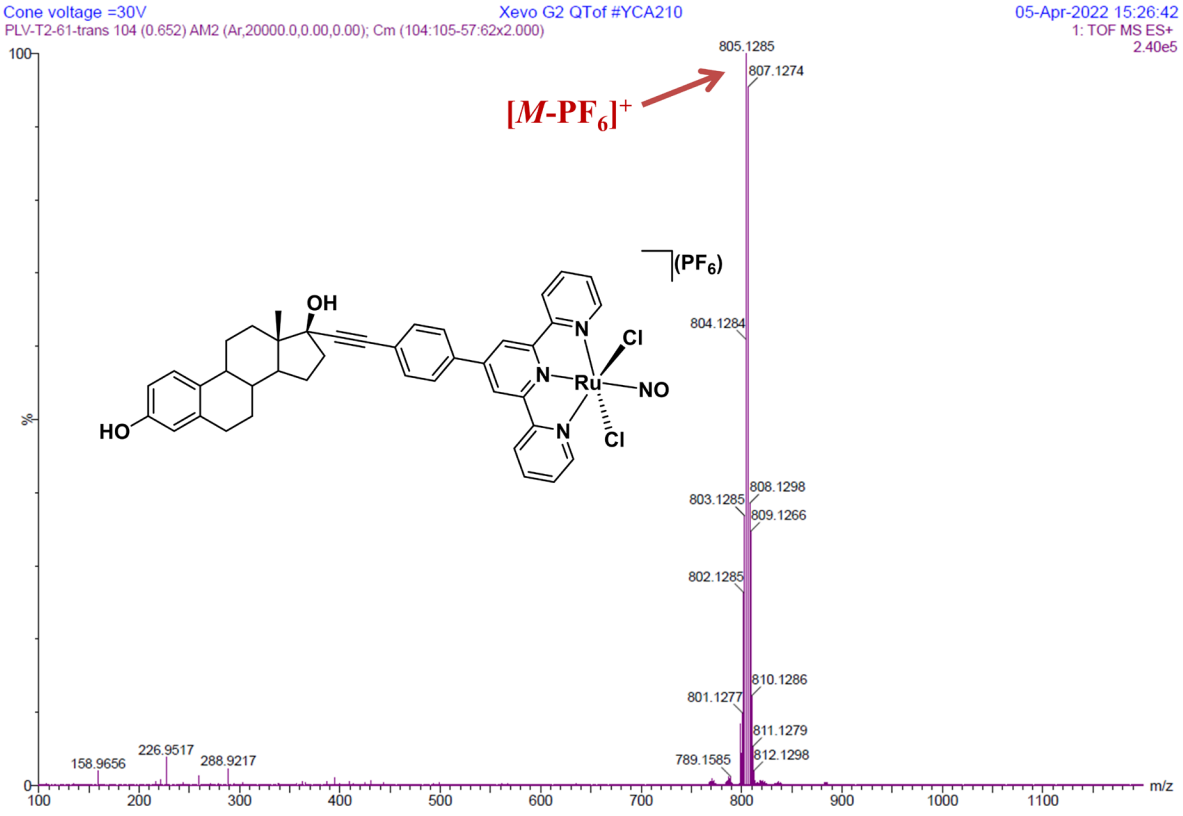
***cis*(Cl,Cl)-[Ru^{II}(EE-Phtpy)(NO)Cl$_2$](PF$_6$) (*cis*-4a)**



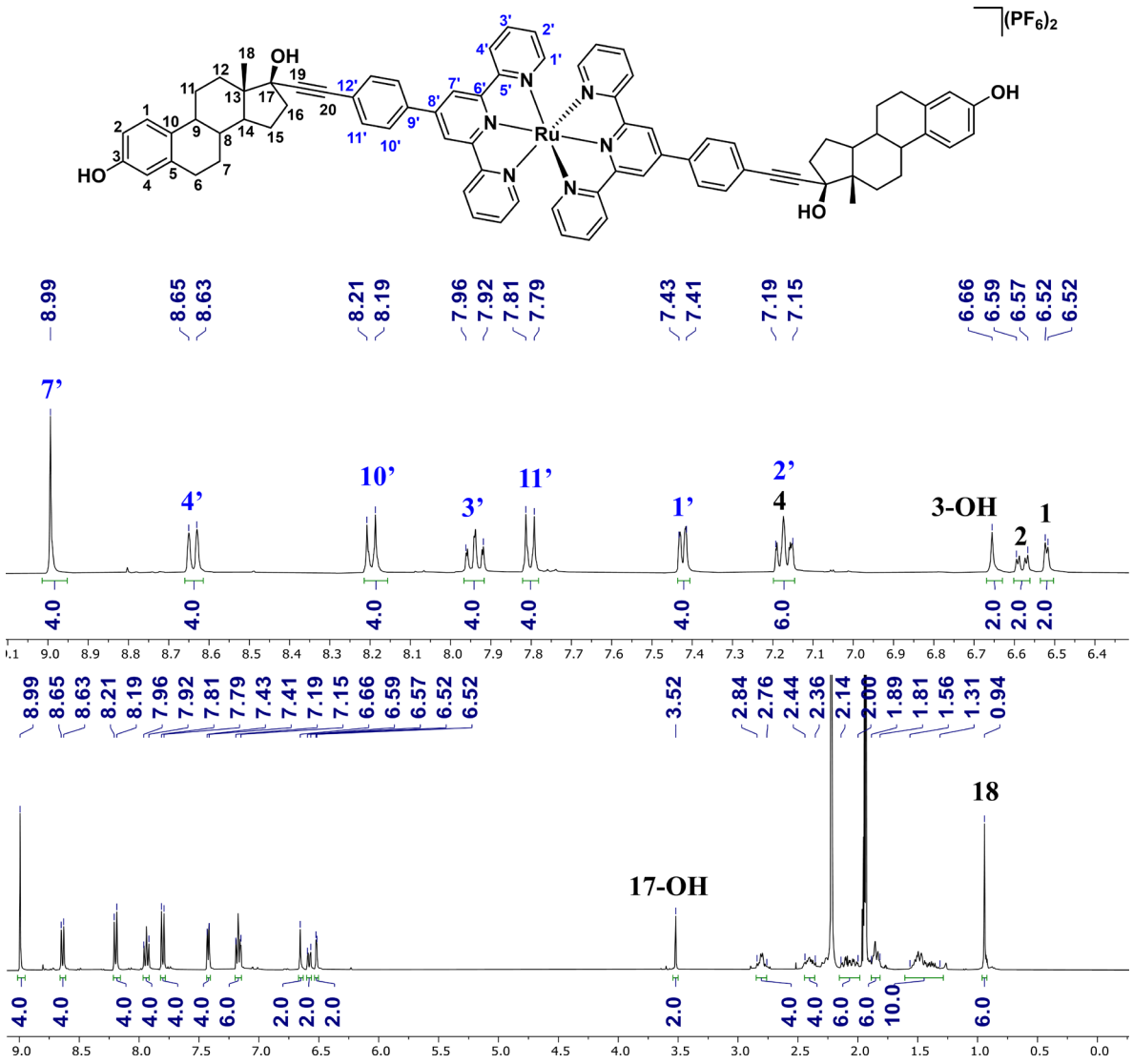


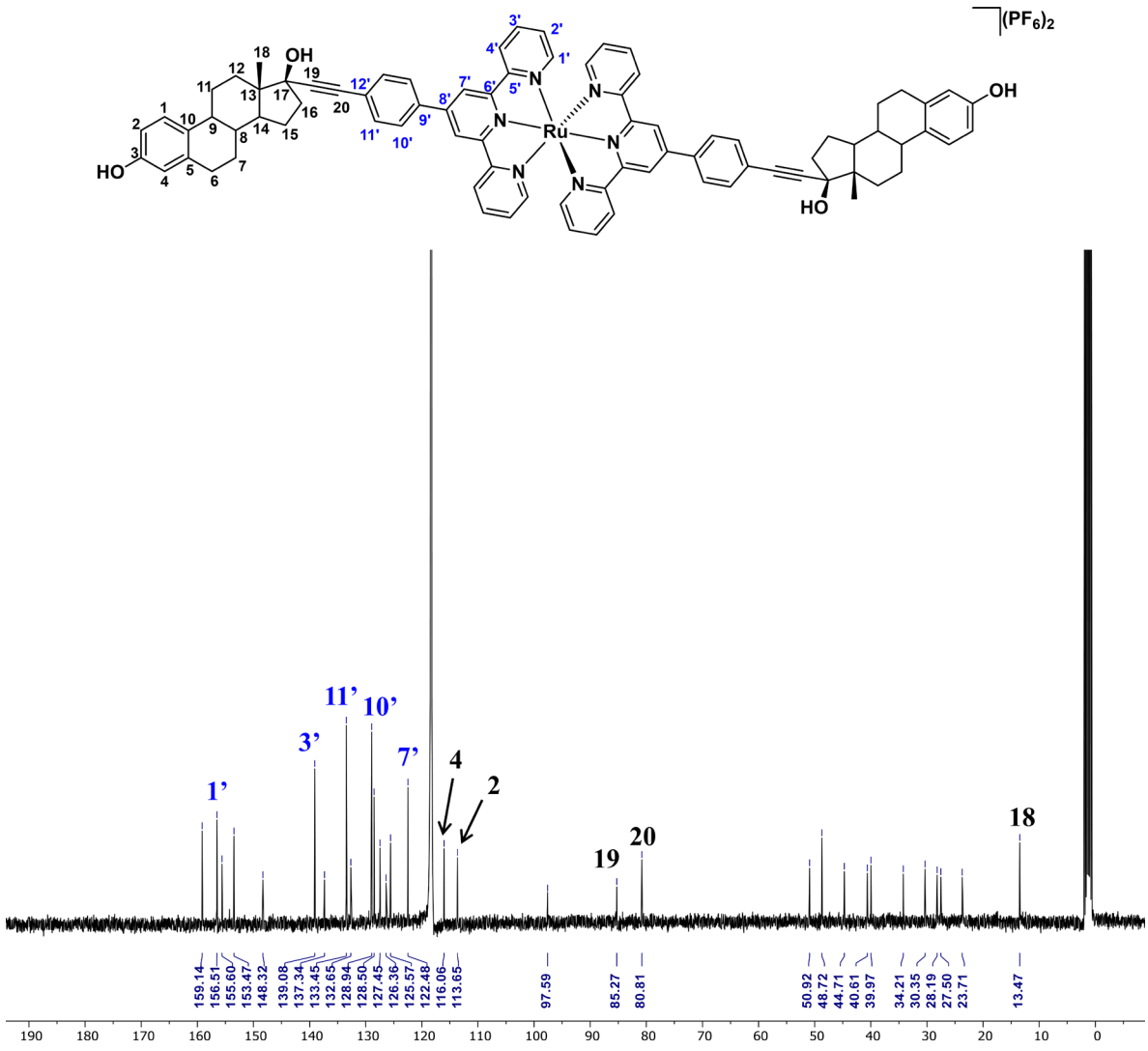
***trans*(Cl,Cl)-[Ru^{II}(EE-Phtpy)(NO)Cl$_2$](PF$_6$) (*trans*-4a)**

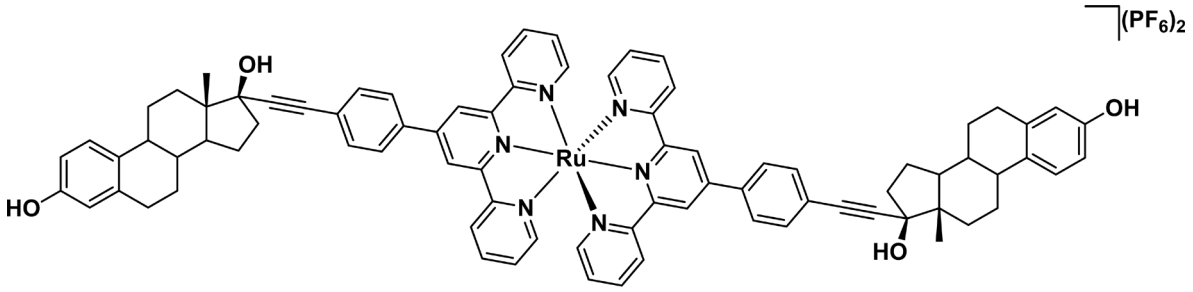


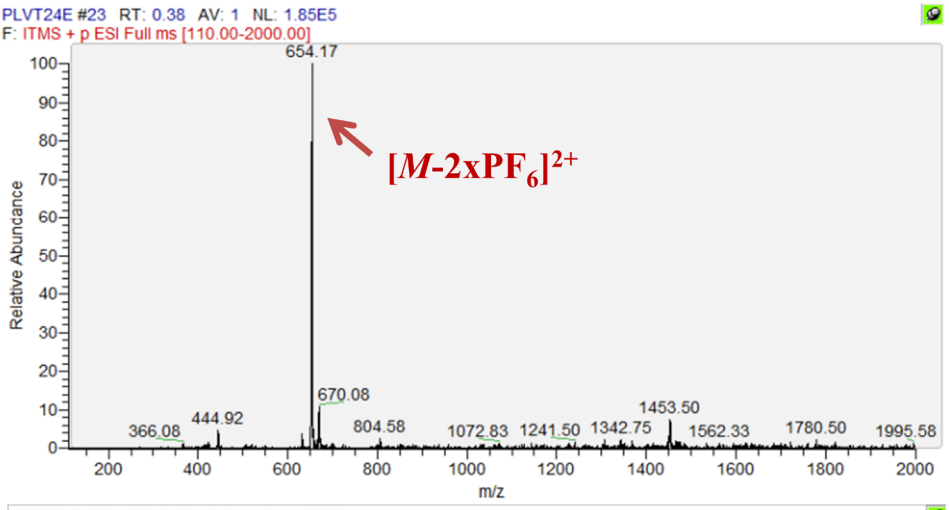

Cone voltage =30V
Xevo G2 QTof #YCA210
05-Apr-2022 15:26:42
PLV-T2-61-trans 104 (0.652) AM2 (Ar,20000.0,0.00,0.00); Cm (104:105-57:62x2.000)
1: TOF MS ES+
2.40e5
[M-PF6]+
(PF6)
OH
HO
N
N
Ru
Cl
NO
Cl
805.1285
807.1274
804.1284
808.1298
803.1285
809.1266
802.1285
810.1286
801.1277
811.1279
789.1585
812.1298
158.9656
226.9517
288.9217
%
m/z

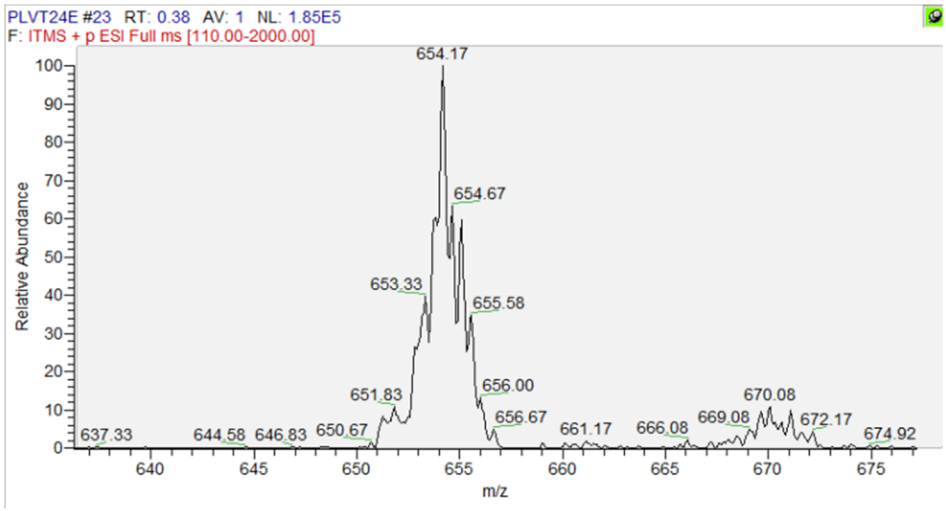
$[Ru^{II}(EE\text{-}Phtpy)_2](PF_6)_2$




(PF6)2
OH
HO
Ru
N
1'
2'
3'
4'
5'
6'
7'
8'
9'
10'
11'
12'
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
1'
3'
11'
10'
7'
4
2
19
20
18
159.14
156.51
155.60
153.47
148.32
139.08
137.34
133.45
132.65
128.94
128.50
127.45
126.36
125.57
122.48
116.06
113.65
97.59
85.27
80.81
50.92
48.72
44.71
40.61
39.97
34.21
30.35
28.19
27.50
23.71
13.47
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0


OH
HO
N
N
Ru
N
N
N
N
OH
HO
(PF6)2


PLVT24E #23 RT: 0.38 AV: 1 NL: 1.85E5
F: ITMS + p ESI Full ms [110.00-2000.00]
654.17
[M-2xPF6]2+
Relative Abundance
m/z
670.08
444.92
366.08
804.58
1072.83
1241.50
1342.75
1453.50
1562.33
1780.50
1995.58


PLVT24E #23 RT: 0.38 AV: 1 NL: 1.85E5
F: ITMS + p ESI Full ms [110.00-2000.00]
654.17
654.67
653.33
655.58
656.00
651.83
656.67
637.33
644.58
646.83
650.67
661.17
666.08
669.08
670.08
672.17
674.92
Relative Abundance
m/z

S3. Miscellaneous Data

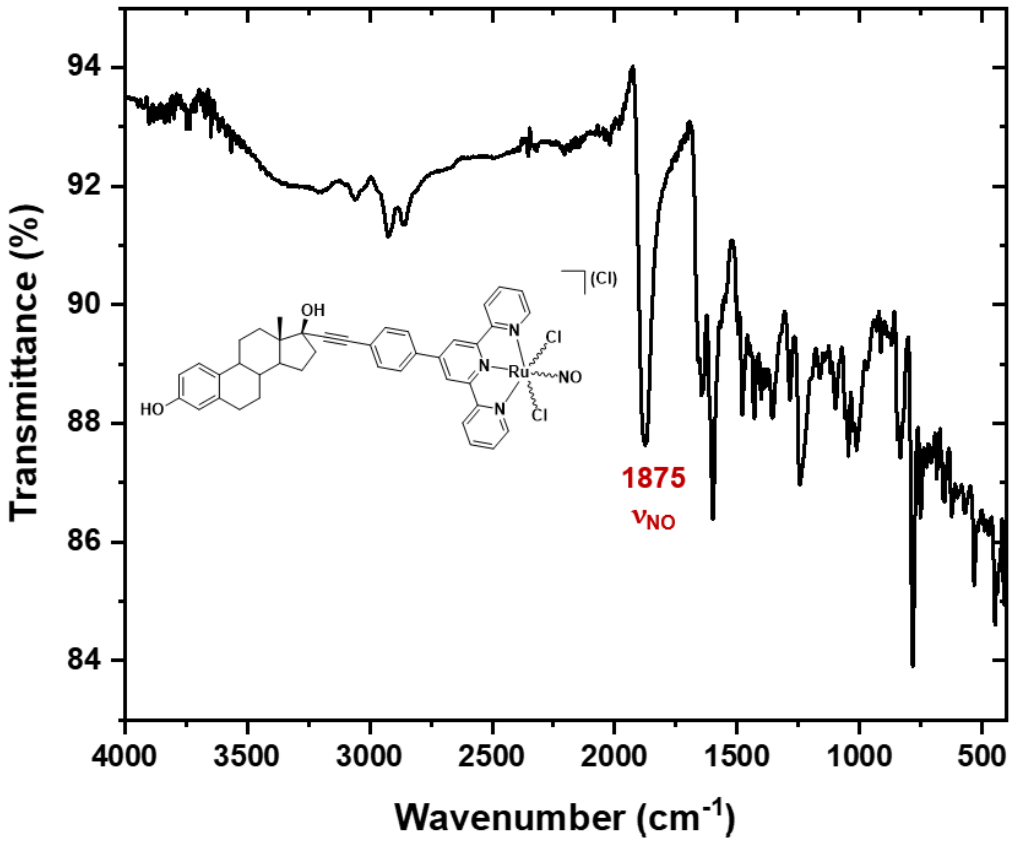


Figure S3. FT-IR (ATR) spectrum for the crude product of the synthesis of ***cis*-4a** and ***trans*-4a**, indicating the observed frequency for the NO stretching vibration.

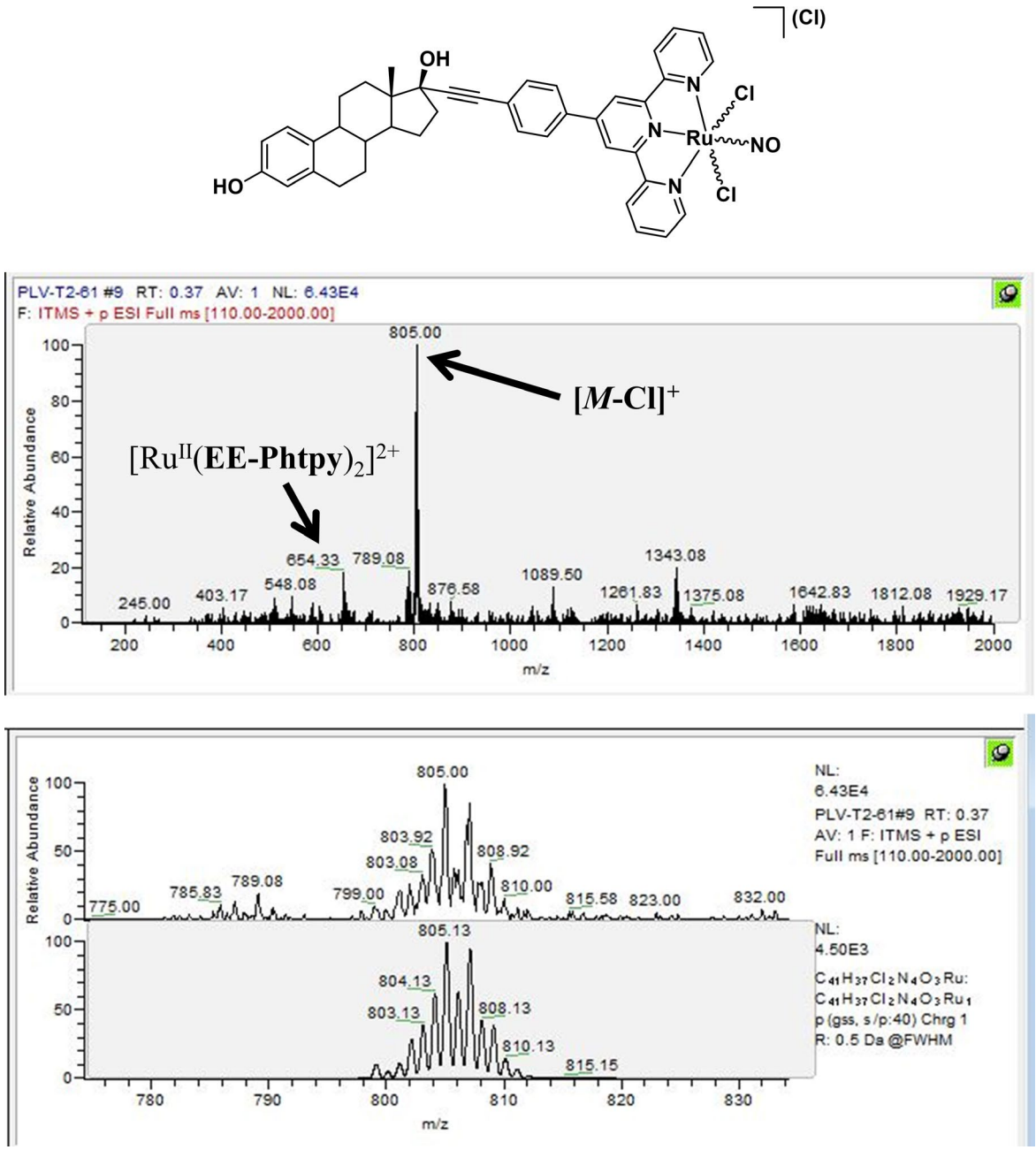
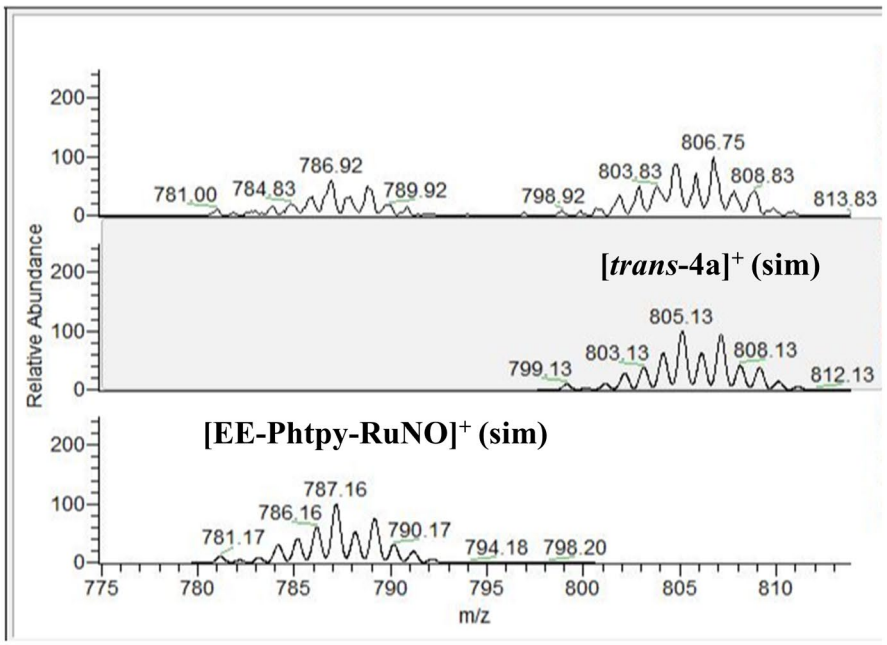
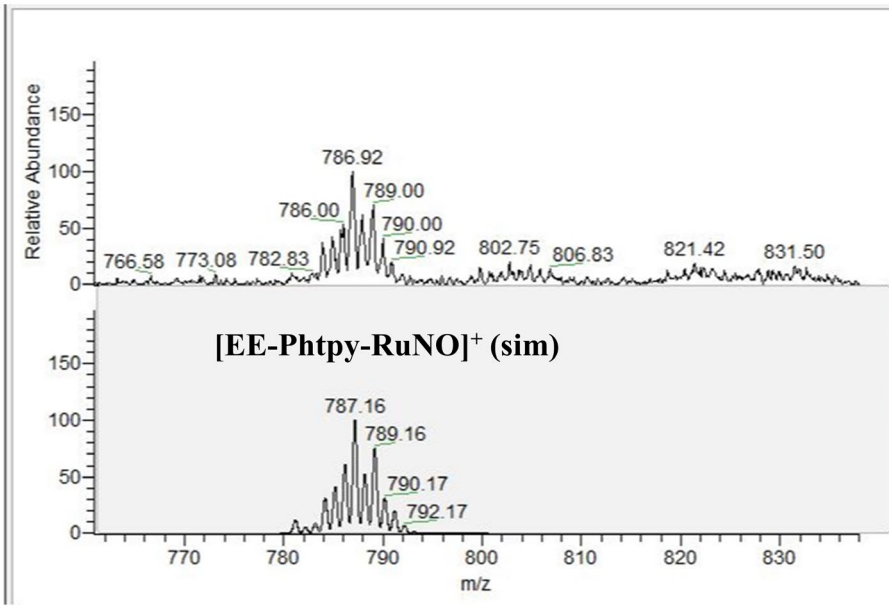


Figure S4. MS (ESI-TOF$^+$) spectrum for the crude product of the synthesis of ***cis*-4a** and ***trans*-4a** where a minor contribution of the homoleptic complex $[Ru^{II}(\mathbf{EE\text{-}Phtpy})_2]^{2+}$ can also be observed. Below is a comparison between the experimental and simulated isotope patterns for the expected $[M\text{-}Cl]^+$ species.



(a)



(b)

Figure S5. Comparison of the MS (ESI-TOF$^+$) spectrum during the hydrolysis of ***trans*-4a** (4.9×10^{-5} M in water + 0.5 % DMSO) into **EE-Phtpy-RuNO**. Spectra are presented at (a) $t = 0$ and (b) $t = 72$ h. Simulated isotope patterns for the cation of both species are included for guidance.

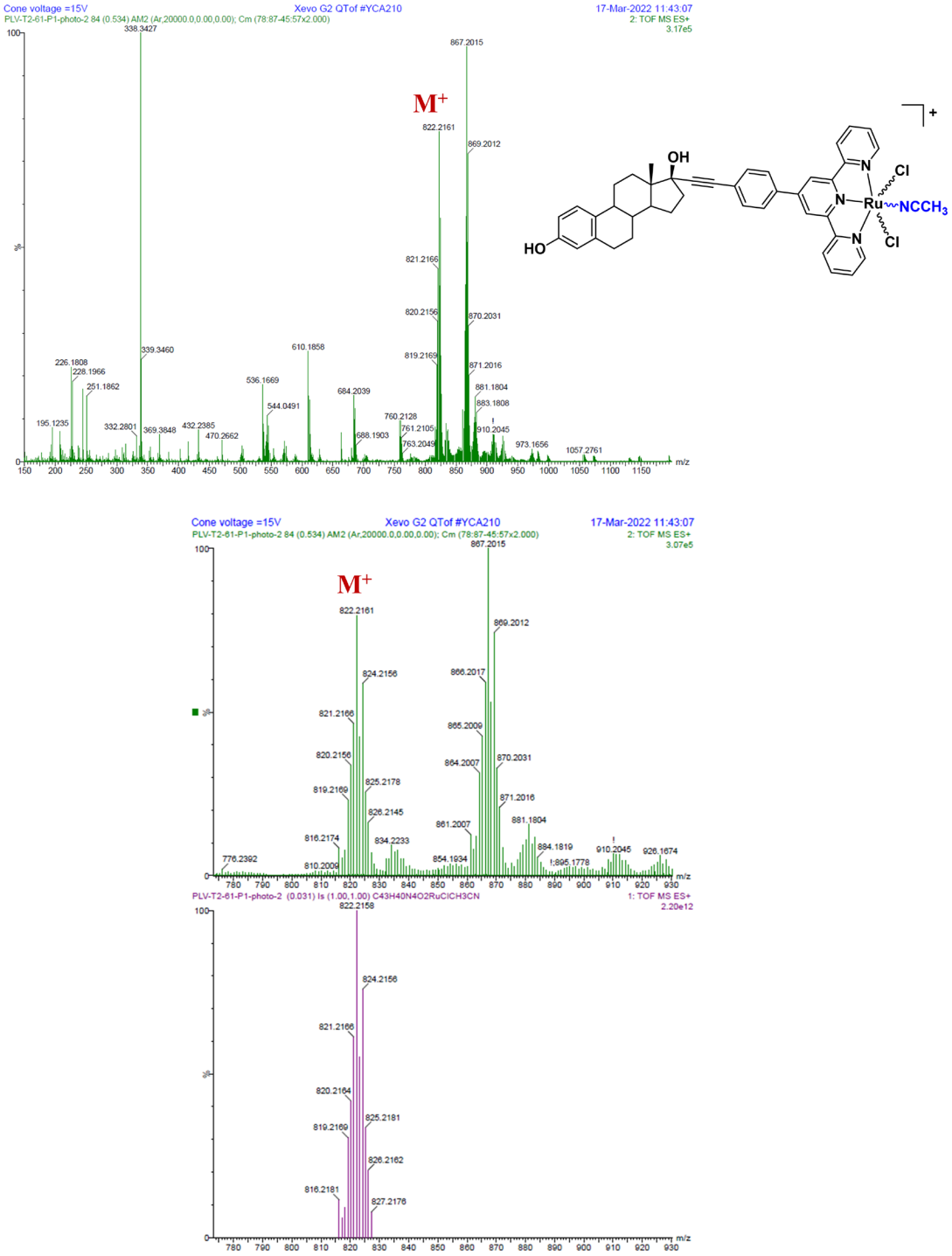


Figure S6. HRMS (ESI-TOF$^+$) spectrum for a photolyzed sample of ***cis*-4a** by irradiation at λ = 365 nm in acetonitrile, showing the formation of the $[Ru^{III}Cl_2$(**EE-Phtpy-RuNO**)(MeCN)$]^+$ solvate photoproduct. Below is a comparison between the experimental and simulated isotope patterns for the expected M^+ species.

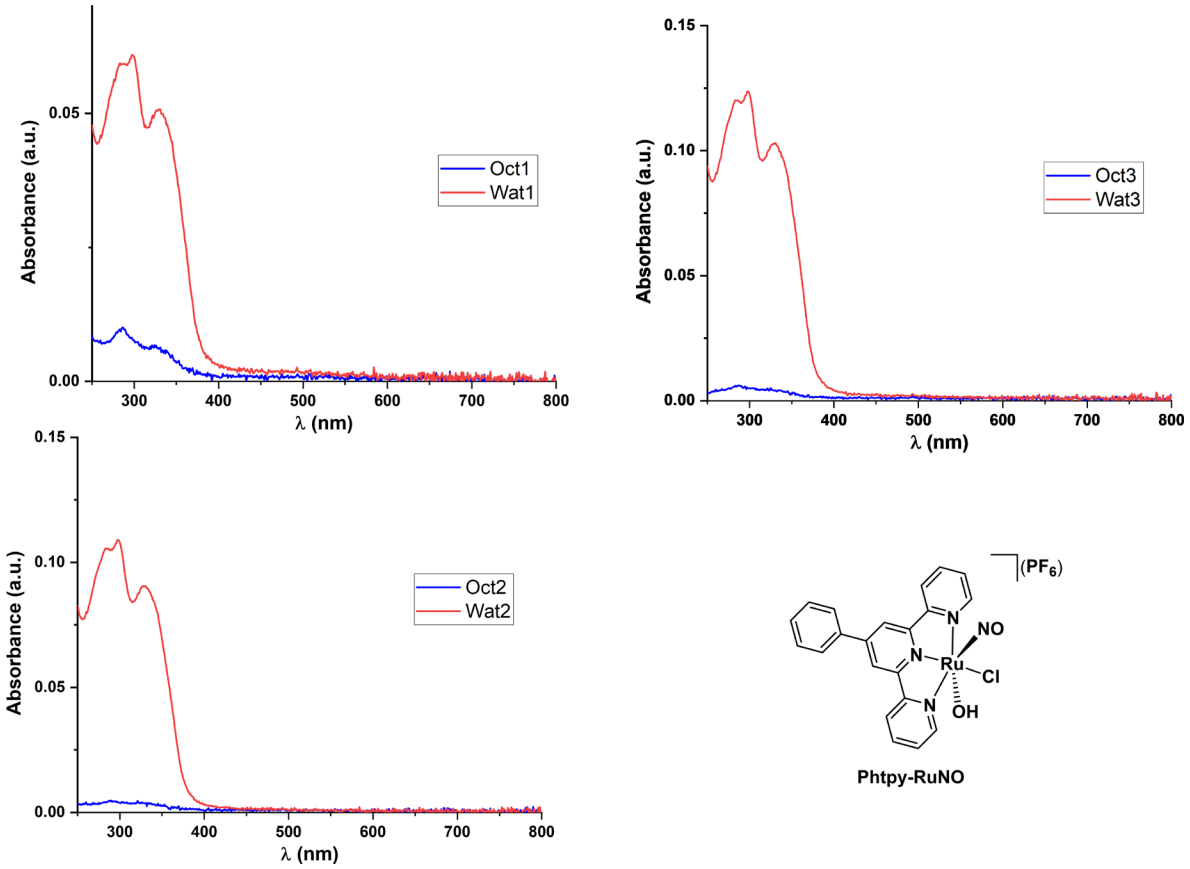


Figure S7. UV-Visible spectra in *n*-octanol (blue line) and water (red line) obtained for the logP measurements of **Phtpy-RuNO**.

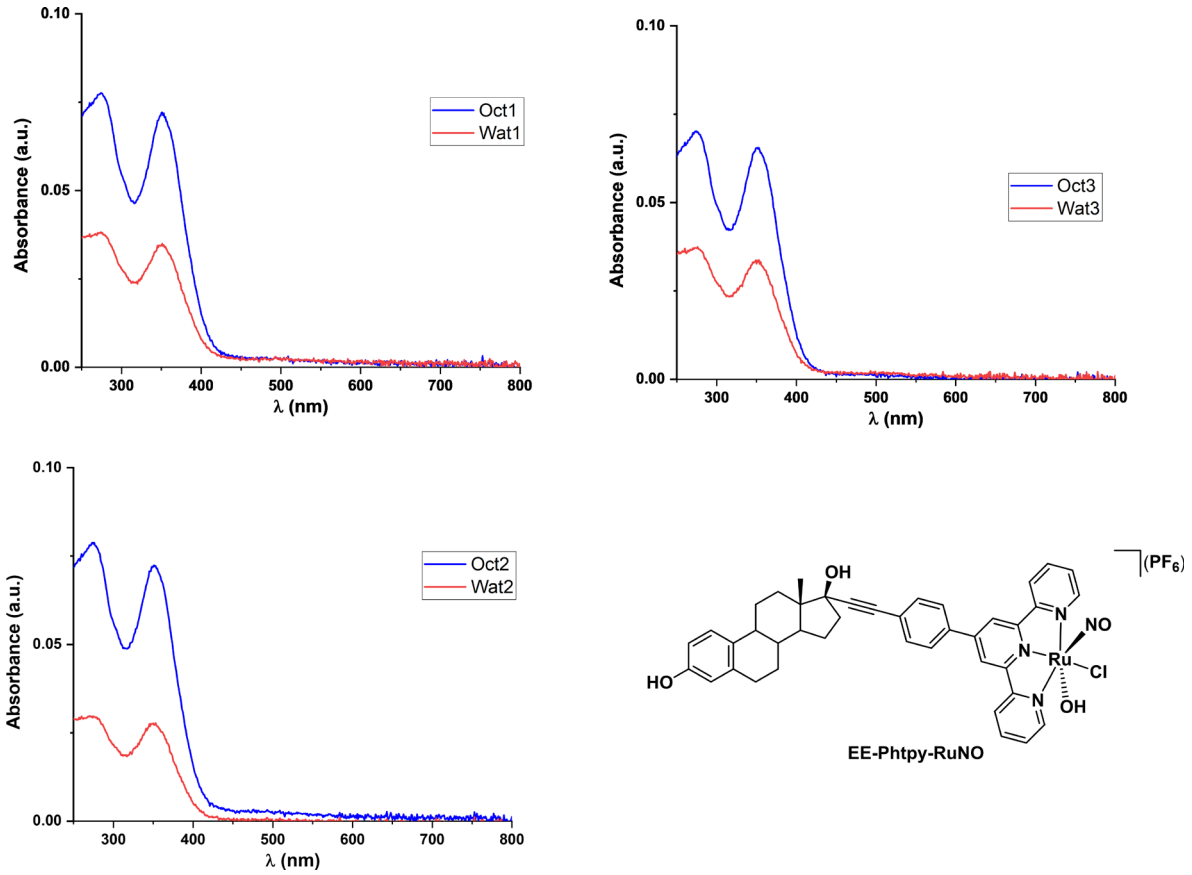


Figure S8. UV-Visible spectra in *n*-octanol (blue line) and water (red line) obtained for the logP measurements of **EE-Phtpy-RuNO**.

Table S1. Details of data collection and refinement.

	***trans*-4a**
Formula	$C_{41}H_{37}Cl_2N_4O_3Ru,F_6P$, $C_4H_{10}O$, C_2H_3N
M ($g.mol^{-1}$)	1065.69
Temperature (K)	100(2)
crystal system	monoclinic
space group	$P2_1$
a (Å)	13.1705(7)
b (Å)	7.6969(4)
c (Å)	27.2166(14)
α (deg)	90
β (deg)	101.3755(17)
γ (deg)	90
volume ($Å^3$)	2704.8(2)
Z	2
Density ($g·cm^{-3}$)	1.308
μ (mm^{-1})	0.482
Crystal size (mm)	0.20 x 0.18 x 0.10
reflns collected/unique (Rint)	84482/13508 (0.051)
Nb. parameters	579
Flack parameter	0.03(3), 6259 Friedel pairs
final *R* indices [$I > 2\sigma(I)$]	0.0400 (9795 refl. $>2\sigma(I)$)
R indices (all data)	0.0431
wR_2 [all data]	0.1029
Residual electron density ($ē.Å^{-3}$)	0.79/-0.46

$R = \Sigma||F_o| - |F_c||/ \Sigma |F_o|$. $wR_2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$.