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Table S1 Cartesian coordinates in xyz format of the optimized geometries of label **1** at ground state

Ir	-1.03476470	0.00675868	-0.00181823
C	-0.84641514	1.37199754	2.72855496
C	-2.13297767	2.51072544	1.09311888
C	-1.09362195	2.35568812	3.67791132
C	-2.90595202	-2.21162983	-0.38381010
C	-3.98693538	-3.08794806	-0.16361452
C	-3.57040662	-0.90224026	1.54062527
C	-4.85442718	-2.87132679	0.90460376
C	-4.64342512	-1.77584749	1.75526629
C	-2.61674517	2.45395838	-0.28322140
C	-3.41773812	3.45600681	-0.86534667
C	-2.67741234	1.19919224	-2.35157721
C	-3.84563115	3.32906094	-2.18512169
C	-3.47373964	2.19750721	-2.92607014
C	1.97405346	0.44575521	0.18743264
C	1.03015264	2.09434894	-1.19030569
C	3.23142749	1.05416965	0.07704457
C	1.74745740	-0.78896852	0.96596893
C	2.26367273	2.71523587	-1.35464285
C	3.40358692	2.20285123	-0.70538333
H	4.07499685	0.62392150	0.59744645
C	2.78588198	-1.54159464	1.52967036
H	2.33264668	3.60179303	-1.97569282
C	0.16050987	-2.30786368	1.79680705
C	2.50541311	-2.70940176	2.25527119
H	3.81929976	-1.24514052	1.39323285
C	1.15554023	-3.08207640	2.38561760
H	0.87930052	-3.97592351	2.93363402
N	0.87866334	0.97714200	-0.43505474
N	0.44202485	-1.18193719	1.09599190
H	0.13102888	2.47254817	-1.65863995
H	-0.88635195	-2.57189884	1.86707375
C	3.61250142	-3.52553301	2.87153266
H	4.59105727	-3.22043843	2.49210503
H	3.62317750	-3.40551596	3.96256793
H	3.47929290	-4.59327493	2.66664292
C	4.73741178	2.92119235	-0.83368356
H	4.86822256	3.23065988	-1.88037671
H	4.66733090	3.85849855	-0.26162138
C	5.99745718	2.16876723	-0.35711025
H	6.82432256	2.88666736	-0.35725281

H	5.87547659	1.84923844	0.68322191
C	6.40149682	0.94545278	-1.22030917
H	5.69224854	0.80488095	-2.05068632
C	6.44232210	-0.37137151	-0.45647139
H	7.38066317	1.11420914	-1.68645362
O	5.87931249	-0.57728387	0.62088935
O	7.11123522	-1.40812086	-1.05762756
H	7.57541034	-1.16512470	-1.88474848
N	-1.34715591	1.44137127	1.46860517
C	-2.22641046	1.29856676	-1.02267540
C	-2.67436827	-1.09590604	0.47331553
H	-5.32215039	-1.60048690	2.58468344
H	-4.15703597	-3.93512350	-0.82084193
H	-3.71176532	4.33200093	-0.29528359
H	-3.81159755	2.09180433	-3.95275891
C	-1.95633451	-2.36625267	-1.48168581
C	-0.01934695	-1.44649518	-2.49527614
C	-1.98648880	-3.36683150	-2.46968013
C	-1.02286589	-3.39658587	-3.47280741
H	-2.77065177	-4.11220075	-2.44706621
H	-1.05179148	-4.16733421	-4.23476402
C	-0.01847223	-2.41756825	-3.48868140
N	-0.95762052	-1.41521470	-1.51494610
C	-1.88742472	3.45419965	3.31701202
C	-2.40328564	3.52706264	2.02672659
H	-2.10164881	4.23744118	4.03544669
H	-3.02312461	4.36483989	1.73522405
H	-3.44109829	-0.05817627	2.21003821
H	-5.68908173	-3.54286429	1.07346424
H	0.74564760	-2.40545448	-4.25586339
H	0.72685005	-0.66529798	-2.46283183
H	-2.41671078	0.33162984	-2.94812973
H	-4.46551277	4.09791686	-2.63321861
H	-0.67936293	2.26115111	4.67390500
H	-0.24873098	0.50055895	2.95524705

Table S2 Cartesian coordinates in xyz format of the optimized geometries of label **2** at ground state

Ir	0.68089558	-0.02076573	-0.05738128
C	0.41667505	1.05842629	-2.89945387
C	1.72629337	2.37976090	-1.42528417
C	0.63492480	1.93404692	-3.95604621
C	2.60958590	-2.13822401	0.52892615
C	3.72734026	-2.96698235	0.33864099
C	3.19773453	-1.00280815	-1.54717294
C	4.58229381	-2.85659818	-0.74530162
C	4.28706310	-1.86019386	-1.67154231
C	2.23107698	2.45944906	-0.05723288
C	3.03330719	3.49006365	0.45861797
C	2.32470212	1.39735402	2.13600540
C	3.49095565	3.51837379	1.76576060
C	3.11727976	2.45237674	2.57918415
C	-2.32546318	0.36469411	-0.26439647
C	-1.39231439	2.14849255	0.94103239
C	-3.58342523	0.97926392	-0.22645273
C	-2.09307892	-0.94770030	-0.90008345
C	-2.62844966	2.77812724	1.03688653
C	-3.76286899	2.20180716	0.43306636
H	-4.42365056	0.49599002	-0.70309669
C	-3.12811562	-1.77218262	-1.35813611
H	-2.70274744	3.72178349	1.56622916
C	-0.49648519	-2.53591232	-1.56708205
C	-2.84100165	-3.01278098	-1.94892312
H	-4.16335133	-1.47525401	-1.23609563
C	-1.48821414	-3.38301615	-2.05172045
H	-1.20696657	-4.33125951	-2.49561801
N	-1.23317237	0.96243271	0.30152650
N	-0.78392135	-1.33952214	-0.99798099
H	-0.49855685	2.57681988	1.37426031
H	0.55172574	-2.79783729	-1.61855778
C	-3.94420792	-3.90495506	-2.45581913
H	-4.91517117	-3.60737625	-2.05162666
H	-4.00931397	-3.85610572	-3.55068745
H	-3.76309385	-4.95157517	-2.19010693
C	-5.09375618	2.93490224	0.46983775
H	-5.22030173	3.37810294	1.46767650
H	-5.01551273	3.79083724	-0.21759305
C	-6.36713866	2.14673574	0.09377456
H	-7.17452603	2.87934313	-0.00819257

H	-6.25399607	1.68486535	-0.89283819
C	-6.81069619	1.06547746	1.11113968
H	-6.20172934	1.11516808	2.02677501
C	-6.72900054	-0.36370962	0.59276200
H	-7.84554522	1.24959972	1.43011452
O	-6.18182179	-0.70763207	-0.45694697
O	-7.28347225	-1.33190620	1.39229786
H	-7.74425080	-0.98860814	2.18537372
N	0.94325990	1.26832008	-1.66645832
C	1.86680280	1.38049316	0.80887650
C	2.33790368	-1.12468223	-0.44399342
C	1.67904001	-2.21220901	1.65158343
C	-0.27951519	-1.23582160	2.57040751
C	1.73796299	-3.10061559	2.74214851
C	0.77496473	-3.04101564	3.74632913
H	2.53987439	-3.82052614	2.78946367
H	0.82731884	-3.72402762	4.58649009
C	-0.25347080	-2.09341581	3.66293533
N	0.65624096	-1.28648546	1.58908280
C	1.42528630	3.06886123	-3.73307907
C	1.96866725	3.29117171	-2.47010215
H	1.61983387	3.77042570	-4.53626610
H	2.58496539	4.15576266	-2.27946126
H	3.04535523	-0.24887353	-2.30821741
H	5.43495103	-3.51054905	-0.85875412
H	-1.01619013	-2.01740811	4.42778773
H	-1.04675893	-0.48320583	2.45732090
H	2.08822803	0.60154994	2.83014720
H	4.10942359	4.32697115	2.12802917
H	0.20176740	1.72719251	-4.92665666
H	-0.17653750	0.16289151	-3.01679374
F	4.01882075	-3.97006650	1.26632038
F	5.12043517	-1.72295735	-2.76998385
F	3.55552855	2.44985106	3.89394204
F	3.40247691	4.56262029	-0.35731204

Table S3 Cartesian coordinates in xyz format of the optimized geometries of label **3** at ground state

Ir	0.92057486	-0.00635716	0.07599937
C	0.84434324	2.39491336	-1.97609959
C	1.42401359	2.85652484	0.28874271
C	0.67690167	3.79366870	-2.24390955
C	0.77711324	1.48871667	-3.06270828
C	0.35984256	4.22180126	-3.55985913
C	0.49258262	1.93909446	-4.34023335
H	0.99719278	0.44955701	-2.88220125
C	0.25757188	3.31144882	-4.59349680
H	0.22223767	5.28330938	-3.74115206
H	0.46408847	1.23113924	-5.16180594
H	0.02539882	3.64510628	-5.59860994
C	2.51250039	-2.31697560	-0.66982379
C	3.47629111	-3.14056846	-1.29149290
C	3.75138247	-0.32973226	-1.30794974
C	4.57340890	-2.57995906	-1.93819872
C	4.69355506	-1.17849161	-1.91170485
C	1.92236866	2.29092821	1.53850082
C	2.43357626	3.10731718	2.57081878
C	2.63005717	0.29444184	2.72436680
C	3.03123889	2.53877009	3.69176119
C	3.13328046	1.13625955	3.72985336
C	-2.11870266	0.51552769	-0.20526986
C	-1.31565609	1.71443109	1.63230956
C	-3.37968408	1.11201460	-0.05912476
C	-1.83761969	-0.47238290	-1.26314258
C	-2.55566393	2.30649592	1.84142021
C	-3.62846881	2.01775690	0.97770876
H	-4.16629670	0.86072413	-0.75504808
C	-2.85115971	-1.05303818	-2.03863306
H	-2.68027810	2.99823213	2.66766963
C	-0.22032497	-1.72156133	-2.39928135
C	-2.54045713	-1.99038660	-3.03308883
H	-3.89079881	-0.80537358	-1.86189641
C	-1.18433844	-2.31530132	-3.20693329
H	-0.87885872	-3.03381603	-3.95950229
N	-1.08689933	0.82855098	0.62986229
N	-0.52748429	-0.81580353	-1.43804865
H	-0.47171132	1.93805871	2.27055105
H	0.82775829	-1.96623416	-2.50449475
C	-3.62053877	-2.61475346	-3.87859801

H	-4.61081113	-2.44424232	-3.44832161
H	-3.61744391	-2.18779477	-4.88994788
H	-3.46886372	-3.69432084	-3.98385505
C	-4.96469701	2.71761162	1.16283137
H	-5.16616847	2.80452209	2.23983090
H	-4.85226254	3.75205868	0.80438522
C	-6.19381856	2.10541263	0.45834864
H	-7.02014741	2.81434407	0.57621911
H	-6.01461581	2.02759128	-0.61906137
C	-6.64319884	0.72356143	0.99654351
H	-6.01639231	0.41346858	1.84679477
C	-6.58013033	-0.39893944	-0.03039549
H	-7.66919791	0.78038984	1.38350743
O	-5.98481852	-0.33948151	-1.10766040
O	-7.20363306	-1.57360860	0.31337637
H	-7.69144150	-1.53790154	1.16163039
N	1.13044630	1.95387617	-0.68645620
C	1.95689469	0.86395917	1.60816801
C	2.59195217	-0.89038036	-0.70367271
H	5.57039998	-0.72641544	-2.36965054
H	3.39284109	-4.22179718	-1.25052061
H	2.39565784	4.18922415	2.49435295
H	3.64198527	0.67763417	4.57476576
C	1.43213056	-2.87590395	0.13483679
C	-0.22551348	-2.40717460	1.77983193
C	1.16773993	-4.27059513	0.25204749
C	0.18451526	-4.72328320	1.09277857
H	1.74323195	-4.96838014	-0.34003779
H	-0.03917403	-5.78265710	1.16690520
C	-0.52390544	-3.80307601	1.91323537
C	-1.47148659	-4.22759930	2.88119344
C	-0.82330372	-1.50133359	2.68997653
C	-2.07090044	-3.31729089	3.72985022
H	-1.69578375	-5.28699978	2.95767985
C	-1.72129909	-1.94877519	3.64365339
H	-0.52379498	-0.46680888	2.65883913
H	-2.78214656	-3.64977920	4.47775503
H	-2.14807288	-1.24201486	4.34788079
N	0.68634622	-1.96937487	0.82293038
C	0.87932173	4.71131693	-1.17720311
C	1.28040933	4.25311494	0.05088720
H	0.74491387	5.77312820	-1.35736983
H	1.48019486	4.94883249	0.85377935
C	3.58688670	3.38714556	4.81369456

H	3.49250154	4.45480061	4.59175193
H	3.06347903	3.19644488	5.75934710
H	4.64903552	3.17600221	4.98704220
C	2.87373951	-1.19181131	2.88362247
H	1.97902445	-1.72381548	3.22630761
H	3.19057852	-1.64312254	1.94131524
H	3.66033345	-1.36988420	3.62387571
C	5.62175112	-3.43476167	-2.61432308
H	5.40820048	-4.50117990	-2.49125383
H	5.67541314	-3.22830264	-3.69081194
H	6.62006380	-3.24534476	-2.20138409
C	4.05934034	1.15316030	-1.30966780
H	3.46918611	1.69824927	-2.05442083
H	3.85912017	1.59815129	-0.33315753
H	5.11485951	1.32078803	-1.54640277

Table S4 Cartesian coordinates in xyz format of the optimized geometries of label **4** at ground state

Ir	1.00677296	0.08742044	-0.04665219
C	1.11691213	-3.04509824	0.79085841
C	2.15636751	-2.33845103	-1.13341291
C	1.60544827	-4.29589370	0.35091495
C	0.41020018	-2.97602901	2.00129378
C	1.39691828	-5.46897919	1.07154679
C	0.19986977	-4.14802905	2.72872202
H	0.04917237	-2.02570247	2.36374684
C	0.68322858	-5.38612776	2.27085731
H	1.78161421	-6.41843858	0.71794091
H	-0.34182748	-4.10038345	3.66696171
H	0.50964928	-6.28407524	2.85304397
C	0.03589302	3.10956701	-0.69877113
C	1.89292938	2.76504820	0.60943459
C	0.35047167	4.46080231	-0.43121459
C	-1.05765279	2.81378828	-1.52621978
C	-0.40041500	5.51310976	-0.94853511
C	-1.81175741	3.86437589	-2.05002389
C	-1.49341582	5.20329496	-1.76335593
H	-0.14315469	6.54327748	-0.73173997
H	-2.65461817	3.64331095	-2.69580788
H	-2.09248307	6.00435104	-2.18149016
C	2.87957463	1.94461359	1.24862464
C	3.96117197	2.43755121	2.00654864
C	3.60194920	-0.32735547	1.62270085
C	4.86161385	1.54051589	2.57114759
C	4.67737481	0.16054743	2.37571782
C	2.58312312	-1.34257320	-2.07312270
C	3.35665261	-1.60619760	-3.22162248
C	2.54208218	1.01328901	-2.59391896
C	3.72093925	-0.55288243	-4.05383654
C	3.31123764	0.75353748	-3.73530309
S	2.51906660	-4.10777924	-1.21308514
S	1.83086517	4.57206206	0.62319025
C	-1.96787108	-0.56242487	-0.11257612
C	-1.04859900	-0.90282943	-2.24292650
C	-3.19017164	-1.09836834	-0.53805873
C	-1.74670275	-0.06329974	1.25747414
C	-2.24997805	-1.41553268	-2.71958157
C	-3.35790438	-1.53437811	-1.85833867
H	-4.00816935	-1.17048887	0.16446854

C	-2.78355977	0.13582049	2.17769059
H	-2.31693058	-1.73402810	-3.75419656
C	-0.17242023	0.69607517	2.82354844
C	-2.50832219	0.62357289	3.46401013
H	-3.81209229	-0.06278463	1.89924266
C	-1.16531042	0.90224414	3.77609158
H	-0.89290382	1.28507315	4.75323357
N	-0.90117452	-0.47810904	-0.96264981
N	-0.44823022	0.21969639	1.58448546
H	-0.17486789	-0.81488424	-2.87437486
H	0.86822537	0.90617687	3.03063394
H	-1.29419350	1.78672802	-1.75897542
C	-3.61220628	0.83904739	4.46719479
H	-4.59691025	0.72941661	4.00599239
H	-3.54107666	0.11268938	5.28679403
H	-3.55013899	1.83683598	4.91549110
C	-4.64590312	-2.16504795	-2.36251294
H	-4.84547806	-1.79048154	-3.37652617
H	-4.46205698	-3.24319497	-2.48335566
C	-5.90760442	-1.99429329	-1.49125433
H	-6.67928069	-2.65271111	-1.90377325
H	-5.71615931	-2.35392502	-0.47493416
C	-6.47110887	-0.55127720	-1.42204404
H	-5.84975259	0.13675424	-2.01609757
C	-6.53416684	0.02780005	-0.01498421
H	-7.47332025	-0.51228079	-1.86739018
O	-5.88073015	-0.38663405	0.94495542
O	-7.33753337	1.12631591	0.16088595
H	-7.86264320	1.37436837	-0.62736985
N	1.43257626	-1.97521530	-0.07236429
N	0.91163997	2.18899259	-0.08857883
C	2.15324240	-0.02491118	-1.72772475
C	2.66836119	0.54759613	1.03790225
H	3.49783773	-1.39860488	1.49240138
H	5.38362676	-0.53890779	2.81284908
H	5.70132848	1.90226120	3.15375679
H	4.09425150	3.50674199	2.14565438
H	3.67116432	-2.61995376	-3.45310521
H	4.32011455	-0.73693108	-4.93848006
H	3.60037978	1.57596258	-4.38276452
H	2.24974561	2.03561545	-2.38191409

Table S5 Cartesian coordinates in xyz format of the optimized geometries of label **5** at ground state

Ir	-0.53607586	0.10296090	-0.01799865
C	-1.74051756	2.50585526	-0.99069146
C	-3.29221257	0.79643113	-1.49802886
C	2.35371495	-0.94971741	-0.10865912
C	1.30051412	-1.77978443	1.80576689
C	3.48792425	-1.72778201	0.16242480
C	2.27355376	-0.05515886	-1.27599251
C	2.41258426	-2.54463944	2.13615831
C	3.54473381	-2.53936494	1.30068825
H	4.32674379	-1.69106158	-0.51701055
C	3.38363978	0.24367211	-2.07740041
H	2.38998764	-3.15019414	3.03568287
C	0.92354184	1.33748472	-2.58336872
C	3.26014087	1.10937934	-3.17252384
H	4.35749990	-0.17050899	-1.84611735
C	1.98932915	1.65721219	-3.41708972
H	1.82891895	2.33612185	-4.24707397
N	1.25998207	-0.98667827	0.70525476
N	1.05003442	0.49754646	-1.52657632
H	0.41159706	-1.78643287	2.42121171
H	-0.06020660	1.75585646	-2.74480177
C	4.44409190	1.43049263	-4.04745314
H	5.38117011	1.11875083	-3.57901341
H	4.36438550	0.91378322	-5.01271657
H	4.50185864	2.50340956	-4.25974309
C	4.73721524	-3.42334573	1.62603680
H	4.90466808	-3.39786444	2.71201718
H	4.45461316	-4.46258267	1.40012940
C	6.05998905	-3.12099355	0.89195506
H	6.75580850	-3.93394062	1.12493783
H	5.90679758	-3.15639880	-0.19160748
C	6.72592078	-1.77148821	1.26545236
H	6.10775809	-1.22126743	1.99164996
C	6.93780997	-0.83639006	0.08258573
H	7.69019032	-1.94483689	1.75982376
O	6.33312526	-0.91205503	-0.98910253
O	7.82813122	0.19229510	0.26484349
H	8.30223826	0.16937931	1.12110399
C	-2.01314341	1.14589250	-0.90994231
C	-2.44567011	0.34031752	2.54429973
C	-3.19717126	-0.48238660	3.42549484

C	-3.93058633	0.03466513	4.49337104
C	-3.92986646	1.41779521	4.68743448
C	-3.20976319	2.26268204	3.82135762
C	-2.47554429	1.73588733	2.76278038
C	-1.76535217	-0.40075359	1.49921207
H	-4.49523481	-0.61676053	5.15090835
H	-4.49705498	1.84258688	5.50887820
H	-3.23205914	3.33549437	3.97939335
H	-1.93327523	2.38873711	2.09399337
C	-1.57484324	-2.60061146	0.47779889
C	-1.61744840	-4.05259835	0.42093467
C	-0.89795914	-2.48430338	-1.82163922
C	-1.30143414	-4.70831840	-0.80733931
C	-1.89170484	-4.84305613	1.56647862
C	-0.68906459	-1.67912226	-2.96321221
C	-1.00355589	-3.89748988	-1.97686045
C	-1.30030807	-6.12248287	-0.84401089
H	-2.07911892	-4.37175803	2.52028438
C	-1.88702838	-6.22704999	1.50098904
C	-0.53783844	-2.24667159	-4.21835372
H	-0.69863228	-0.60872324	-2.84603786
C	-0.83276830	-4.44757778	-3.26936783
C	-1.59589351	-6.87143251	0.28434333
H	-1.05519696	-6.63778742	-1.76377758
H	-2.09920299	-6.81032180	2.39006198
C	-0.59329912	-3.64428954	-4.37344869
H	-0.39671124	-1.60860636	-5.08413256
H	-0.91515628	-5.51779378	-3.41117927
H	-1.59106244	-7.95482853	0.23083297
H	-0.47451253	-4.09058653	-5.35447888
C	-2.00507625	-1.76720534	1.56865154
N	-1.09011212	-1.87969109	-0.57112081
S	-3.09882884	-2.23802695	2.97382484
S	-3.06937706	3.46020497	-1.83607941
C	-3.98680575	1.90805033	-2.04590012
C	-5.23805384	1.78817033	-2.65061407
C	-3.92304908	-0.46637589	-1.55825707
C	-5.82857137	0.52360912	-2.70257439
H	-5.74523130	2.65393074	-3.06137895
C	-5.17471378	-0.59566579	-2.15284190
H	-3.42985903	-1.32625685	-1.12867613
H	-6.80339265	0.40737925	-3.16420172
H	-5.65463711	-1.56759489	-2.19030531
C	-0.61466077	3.02856998	-0.26505651

C	0.88252692	2.48322721	1.52859301
C	-0.08940942	4.38273605	-0.32889468
C	1.38191755	3.81727801	1.58501479
C	1.24443191	1.56911290	2.54273497
C	-0.51155841	5.30757886	-1.31809432
C	0.93821829	4.77231596	0.58221253
C	2.27253451	4.15964635	2.62984634
H	0.79346789	0.59133501	2.53802985
C	2.10846866	1.93818369	3.56154371
C	0.03405832	6.57918385	-1.39077014
H	-1.24729922	5.01880337	-2.05436167
C	1.48001759	6.07500805	0.48235508
C	2.64175907	3.23988177	3.59917136
H	2.65711118	5.16962906	2.69546538
H	2.35392997	1.22651116	4.34281065
C	1.03295886	6.96789999	-0.47925491
H	-0.30322387	7.26830053	-2.15689863
H	2.26728808	6.38507888	1.15736068
H	3.31638210	3.53233691	4.39624113
H	1.46313217	7.96203846	-0.53582708
N	-0.03215229	2.09580924	0.53905524

Table S6 Cartesian coordinates in xyz format of the optimized geometries of **Ru-based Label** at ground state

C	-1.82989240	0.18967001	-3.02877240
C	-2.32045403	-1.83843047	-1.93425065
C	-2.39867733	-0.26499895	-4.21645834
C	-2.51084731	1.12614906	2.15873340
C	-3.61194658	1.60229254	2.88438680
C	-3.87606450	0.82027719	0.26185222
C	-4.86507201	1.68549107	2.27576283
C	-4.99898630	1.28767148	0.94061671
C	-2.22533112	-2.59003394	-0.67324174
C	-2.74805053	-3.87707125	-0.48616841
C	-1.43434670	-2.56981631	1.54659907
C	-2.60432856	-4.51414447	0.74733535
C	-1.93458906	-3.84898687	1.78032580
C	1.77439581	0.54010460	-1.24603281
C	1.50368057	-1.76208921	-0.86828601
C	3.10282179	0.33167338	-1.61884890
C	1.12334567	1.86082201	-1.21569544
C	2.82173842	-2.01583236	-1.23595031
C	3.66899910	-0.95194912	-1.58088597
H	3.72287030	1.17374685	-1.89954310
C	1.73341501	3.04398993	-1.64900080
H	3.18873683	-3.03585731	-1.22752664
C	-0.82610176	3.05387124	-0.67171053
C	1.05557413	4.27030465	-1.59337208
H	2.74383869	3.02071263	-2.03689658
C	-0.25897753	4.25173928	-1.08929755
H	-0.83657204	5.16664648	-1.02269954
N	0.98734347	-0.51066943	-0.83783224
N	-0.16020607	1.87162586	-0.73011335
H	0.84196570	-2.56132885	-0.56513534
H	-1.83337133	3.01612696	-0.28026033
C	1.70335903	5.55324987	-2.04286398
H	2.66312772	5.37303348	-2.53310104
H	1.06010826	6.09799223	-2.74265163
H	1.88300417	6.21803413	-1.18870386
C	5.14219450	-1.15706729	-1.85273224
H	5.34354635	-2.22262534	-2.01515870
H	5.41039053	-0.64434635	-2.78543394
C	6.08736979	-0.62042353	-0.73786021
H	7.10527737	-0.64655606	-1.14195432
H	5.85677345	0.43024549	-0.52813988
C	6.09002314	-1.40820031	0.58564928

H	6.10816217	-2.49096997	0.39090408
C	4.93661062	-1.10095973	1.52386042
H	7.02000506	-1.18708680	1.13061805
O	4.05952500	-0.25740852	1.32302990
O	4.88422256	-1.82955844	2.68890979
H	5.62946028	-2.45193638	2.81963937
N	-1.78754481	-0.57169828	-1.90561305
C	-1.15226452	1.00236125	2.71073712
C	1.06906000	0.34032722	2.27795456
C	-0.79983597	1.37220347	4.01500301
C	0.51806987	1.21444378	4.45181618
H	-1.54205311	1.78220607	4.68739326
H	0.79526138	1.49819012	5.46023247
C	1.46619313	0.69098289	3.56815655
N	-0.21164464	0.48437472	1.85162260
C	-2.94447969	-1.55299462	-4.25671138
C	-2.90257578	-2.34165592	-3.10587408
H	-3.39214326	-1.93639403	-5.16586466
H	-3.31729989	-3.34092111	-3.12549774
H	-3.93214895	0.50149169	-0.76963769
H	-5.71942857	2.05208881	2.83228146
H	2.50114238	0.54834338	3.85182047
H	1.79172603	-0.05294078	1.57879154
H	-0.91052562	-2.01974328	2.31562537
H	-3.00791994	-5.50816111	0.89916877
H	-2.41086503	0.37733349	-5.08835626
H	-1.39579501	1.17644263	-2.95109496
H	-5.95439295	1.33640884	0.43292656
H	-3.49624955	1.90470168	3.91682923
H	-3.26662641	-4.37979298	-1.29194358
H	-1.80223793	-4.30946642	2.75160485
N	-1.57190789	-1.94415738	0.34942567
N	-2.65391422	0.73869841	0.84778990
Ru	-0.90765459	0.00897902	-0.08134916

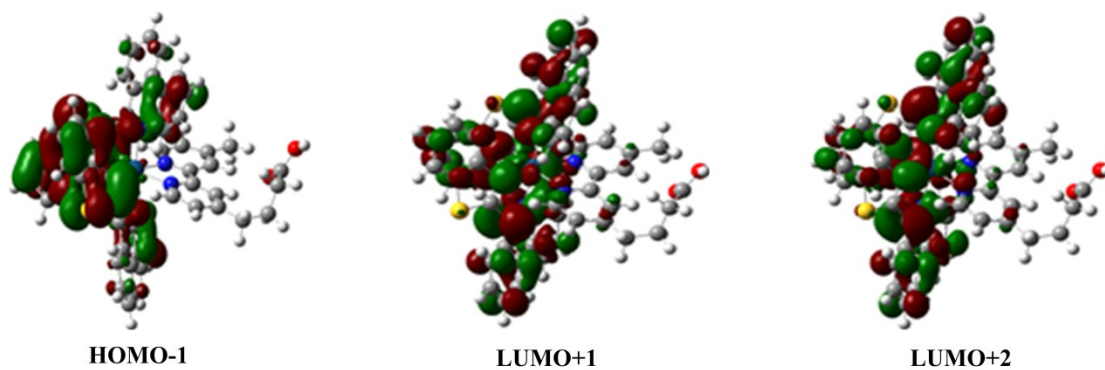


Figure S1. The electron distributions on frontier orbitals of **Label 5** based on the optimization of ground state using DFT calculations.

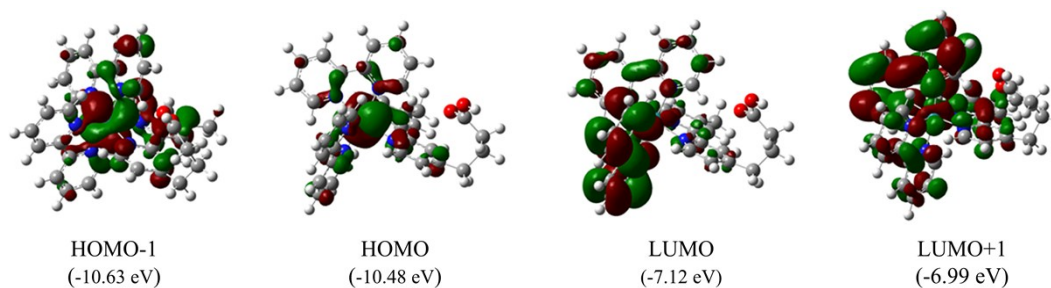


Figure S2. The electron distributions on frontier orbitals of **Ru-based Label** based on the optimization of ground state using DFT calculations.

Table S7. TD-DFT calculated transition wavelength, oscillator strength (f) and molecular orbitals involved in the lowest-energy transition of **Ru-based Label**.

Complex	State	λ_{max} [nm]	f	Assignments
Ru-based Label	T_1	539	0.0000	HOMO $\rightarrow$ LUMO (57.16%)
				HOMO-1 $\rightarrow$ LUMO (10.93%)
				HOMO $\rightarrow$ LUMO+1 (34.91%)
	S_1	509	0.0009	HOMO $\rightarrow$ LUMO (64.25%)
				HOMO $\rightarrow$ LUMO+1 (26.87%)

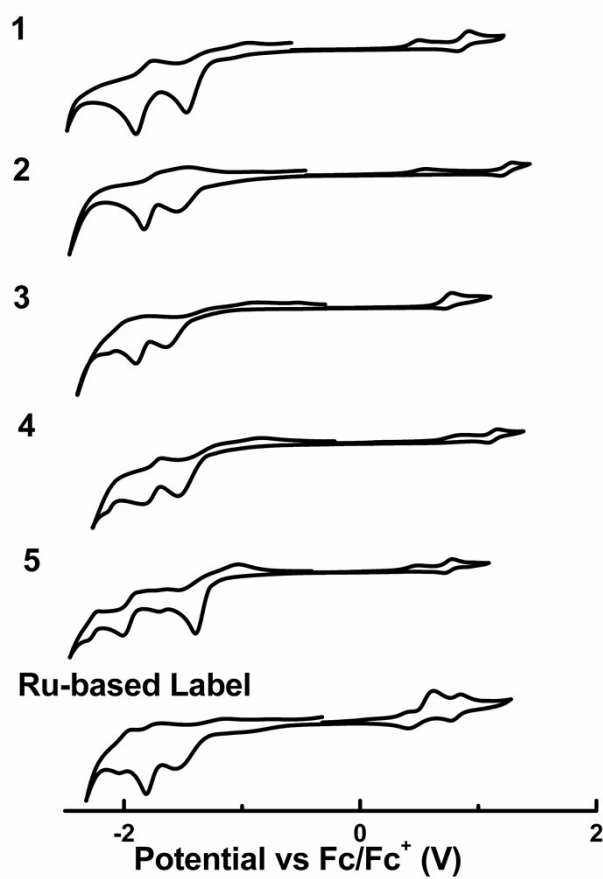


Figure S3. Cyclic voltammetry of 1 mM ECL labels with 0.1 M TBAPF₆ in acetonitrile solution. Pt electrode area: 3.14 mm², scan rate: 0.1 V/s.

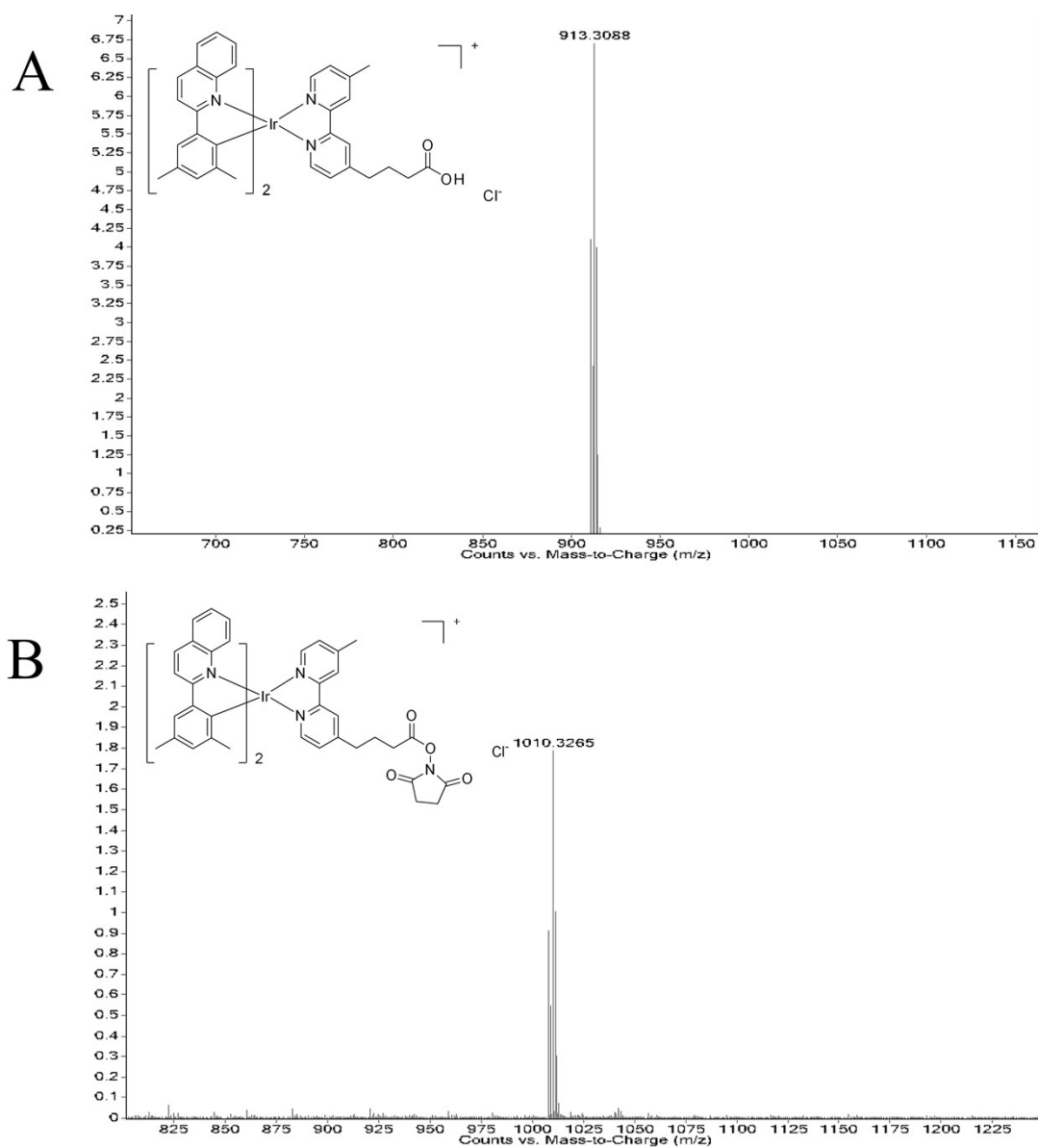


Figure S4. Tof-Ms spectra of Label **3** (A) and its N-HydroxySuccinimide(NHS) ester form (B).

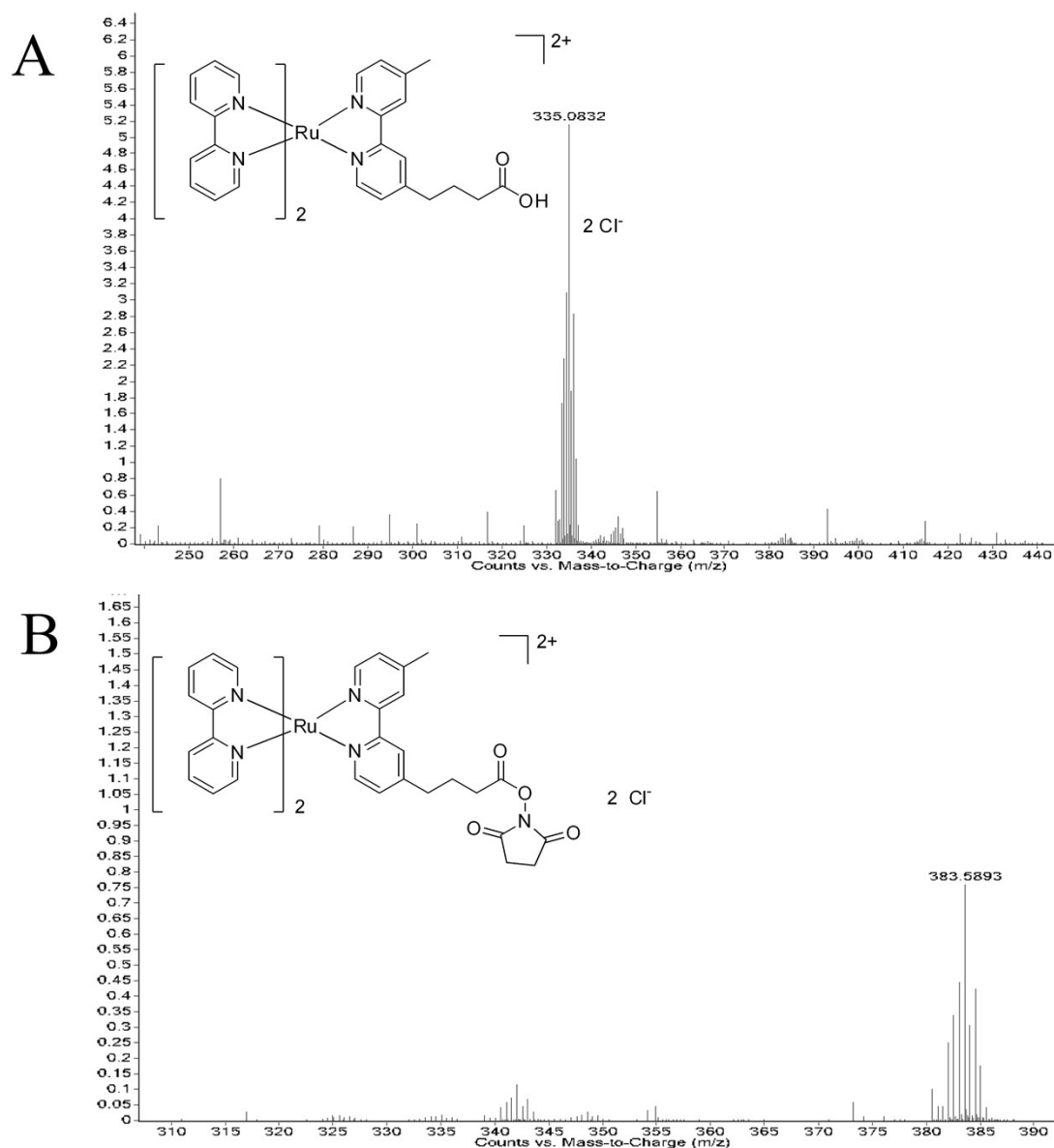


Figure S5. Tof-Ms spectra of **Ru-based Label** (A) and its N-HydroxySuccinimide(NHS) ester form (B).