Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supplementary Information

β-Diketiminate-Supported Iridium Photosensitizers with Increased Excited-State Reducing Power

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Contents

Table S1. Crystallographic Details for complexes **1** and **3**–**6.**

	1	**3**	**4·C_5H_{12}**	**5**	**6**
CCDC	2071495	2071496	2071497	2071498	2071499
Crystal data					
Chemical formula	$C_{43}H_{51}IrN_{10}$	$C_{47}H_{43}IrN_6O_2$	$C_{47}H_{45}IrN_8$	$C_{50}H_{51}IrN_6$	$C_{45}H_{51}IrN_6$
M_r	900.13	916.07	914.11	928.16	868.11
Crystal system, space group	Monoclinic, $P2_1/n$	Monoclinic, $C2/c$	Monoclinic, $P2_1/c$	Orthorhombic, *Pbca*	Orthorhombic, *Pbca*
Temperature (K)	123	296	123	123	123
a, b, c (Å)	9.6392 (13), 21.201 (3), 19.632 (3)	29.266 (3), 13.6816 (14), 21.192 (2)	15.6120 (13), 13.5250 (12), 21.1367 (18)	20.975 (3), 14.266 (2), 27.118 (4)	21.013 (7), 14.522 (5), 28.498 (9)
β (°)	100.559 (1)	90.712 (2)	104.298 (1)	90	90
V (Å^3)	3944.0 (9)	8484.7 (15)	4324.8 (6)	8114 (2)	8696 (5)
Z	4	8	4	8	8
μ (mm^{-1})	3.43	3.19	3.13	3.34	3.11
Crystal size (mm)	0.26 × 0.11 × 0.04	0.37 × 0.12 × 0.08	0.33 × 0.16 × 0.09	0.28 × 0.28 × 0.13	0.34 × 0.12 × 0.05
Data collection					
T_{min}, T_{max}	0.548, 0.746	0.544, 0.746	0.530, 0.746	0.602, 0.746	0.611, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	56520, 9053, 7540	26017, 9725, 8159	61087, 9953, 8113	49198, 9366, 7535	49384, 9583, 6613
R_{int}	0.052	0.024	0.036	0.046	0.063
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.649	0.650	0.651	0.651	0.641
Refinement					
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.056, 1.05	0.026, 0.077, 1.09	0.023, 0.066, 1.17	0.028, 0.070, 1.04	0.031, 0.088, 1.03
No. of reflections	9053	9725	9953	9366	9583
No. of parameters	515	535	511	540	474
No. of restraints	94	103		171	
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.00, -0.55	1.53, -0.48	1.09, -1.25	1.24, -0.94	1.08, -0.59

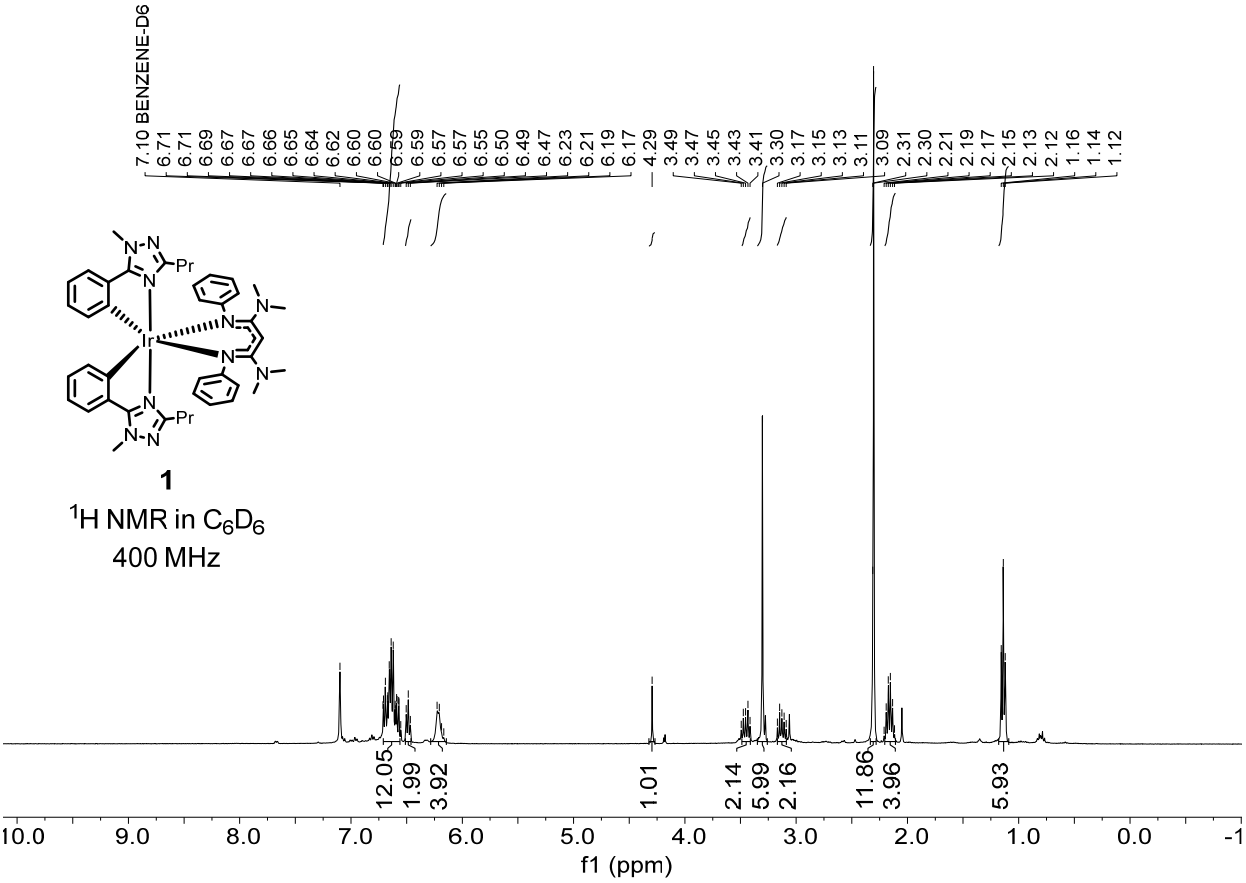


Fig. S1. ^{1}H NMR spectrum of Ir(ptz)$_2$(NacNac^{NMe2}) (**1**), recorded at 400 MHz in C_6D_6.

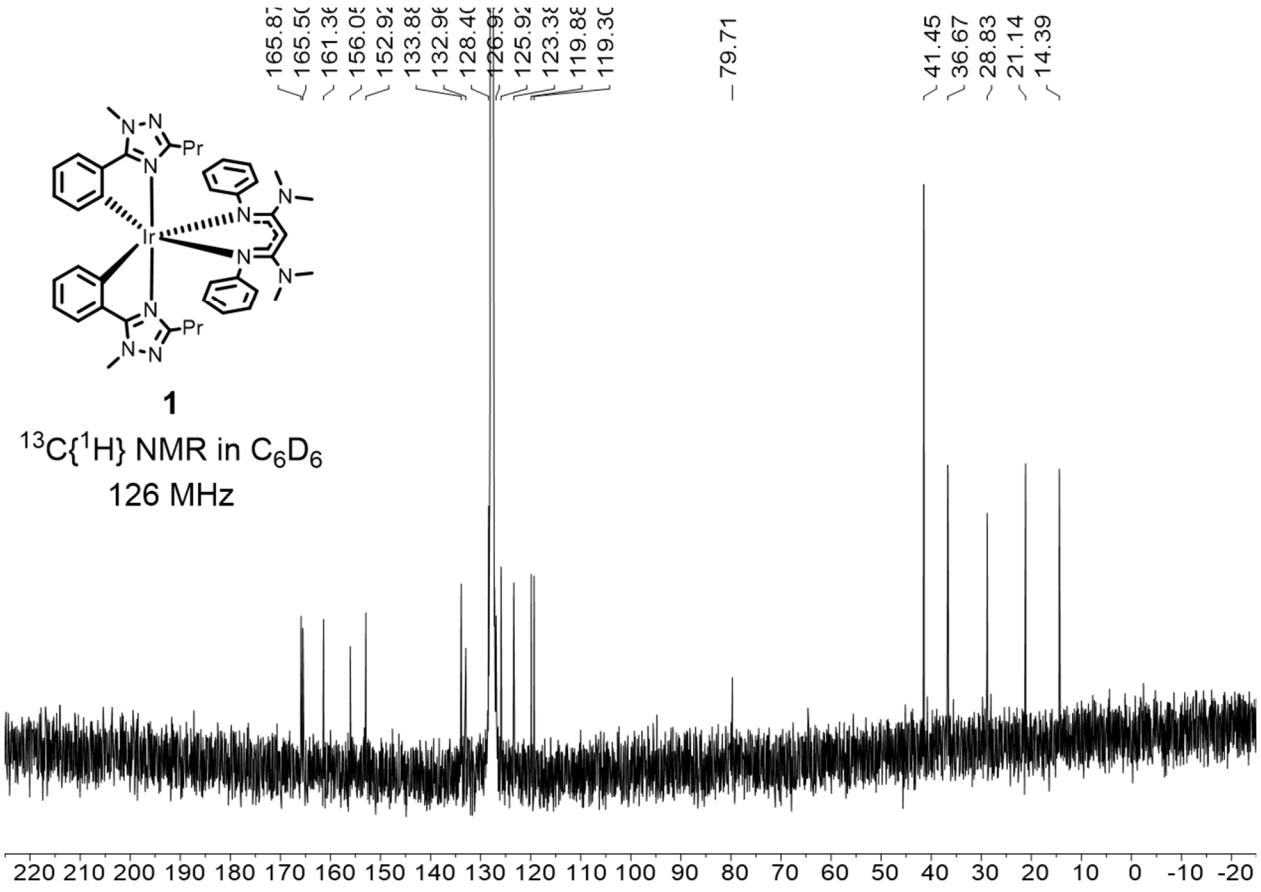


Fig. S2. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(ptz)_2(NacNac^{NMe2})$ (**1**), recorded at 126 MHz in C_6D_6.

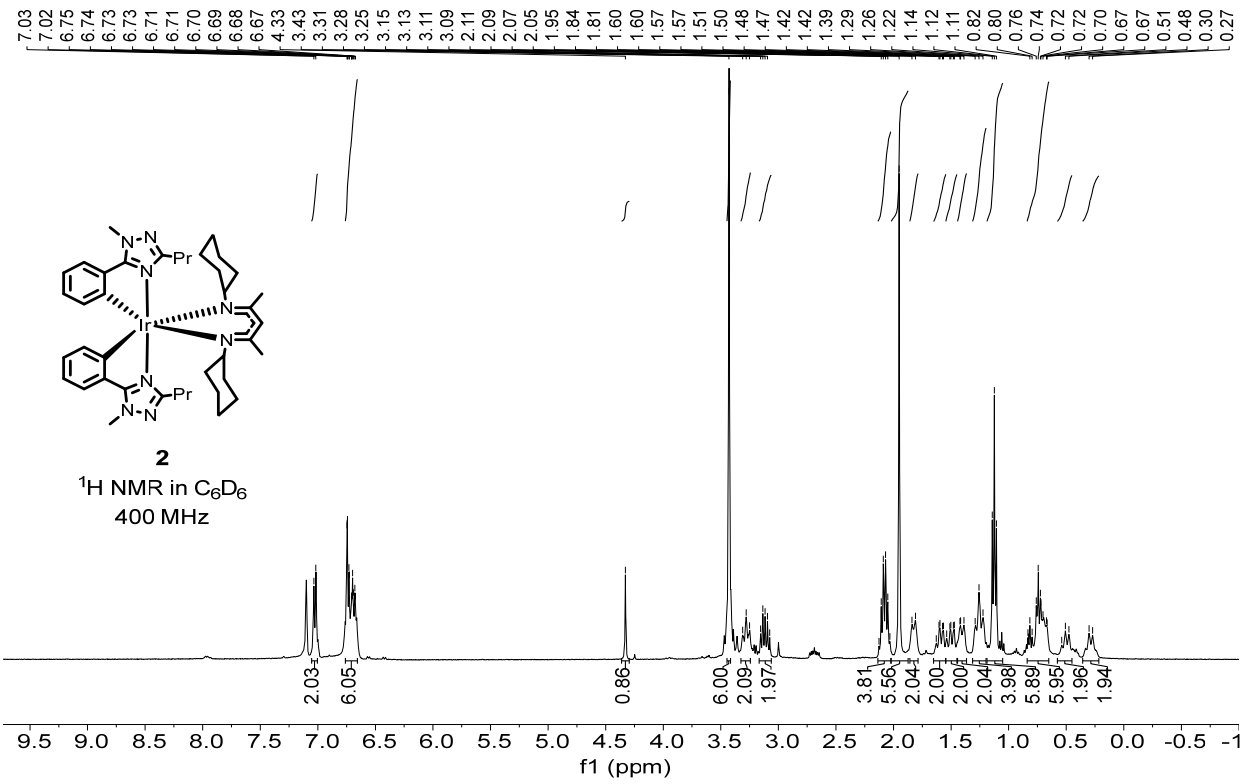


Fig. S3. ^{1}H NMR spectrum of Ir(ptz)$_2$(NacNac^{Cy}) (**2**), recorded at 400 MHz in C_6D_6.

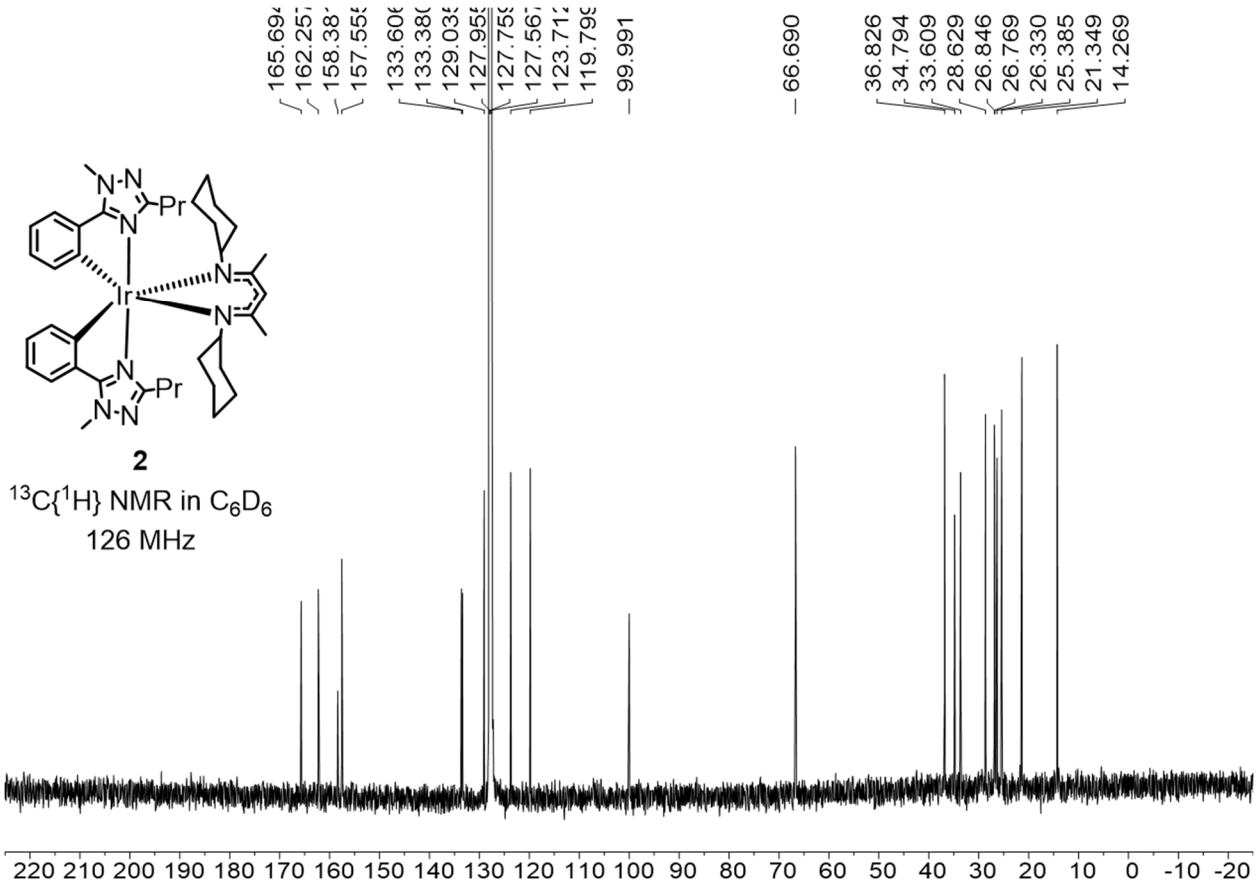


Fig. S4. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(ptz)_2(NacNac^{Cy})$ (**2**), recorded at 126 MHz in C_6D_6.

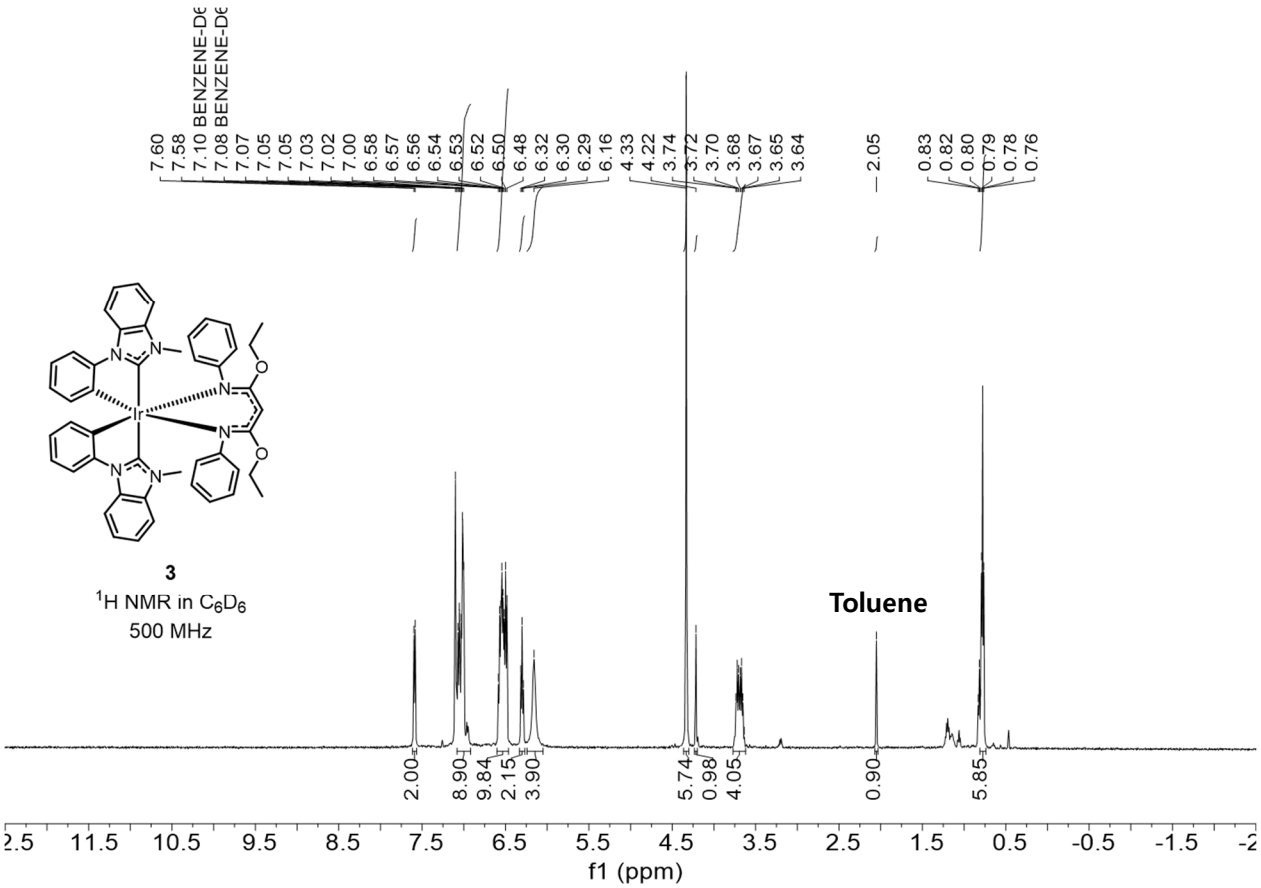


Fig. S5. ^{1}H NMR spectrum of Ir(pmb)$_2$(NacNac^{OEt}) (**3**), recorded at 500 MHz in C_6D_6.

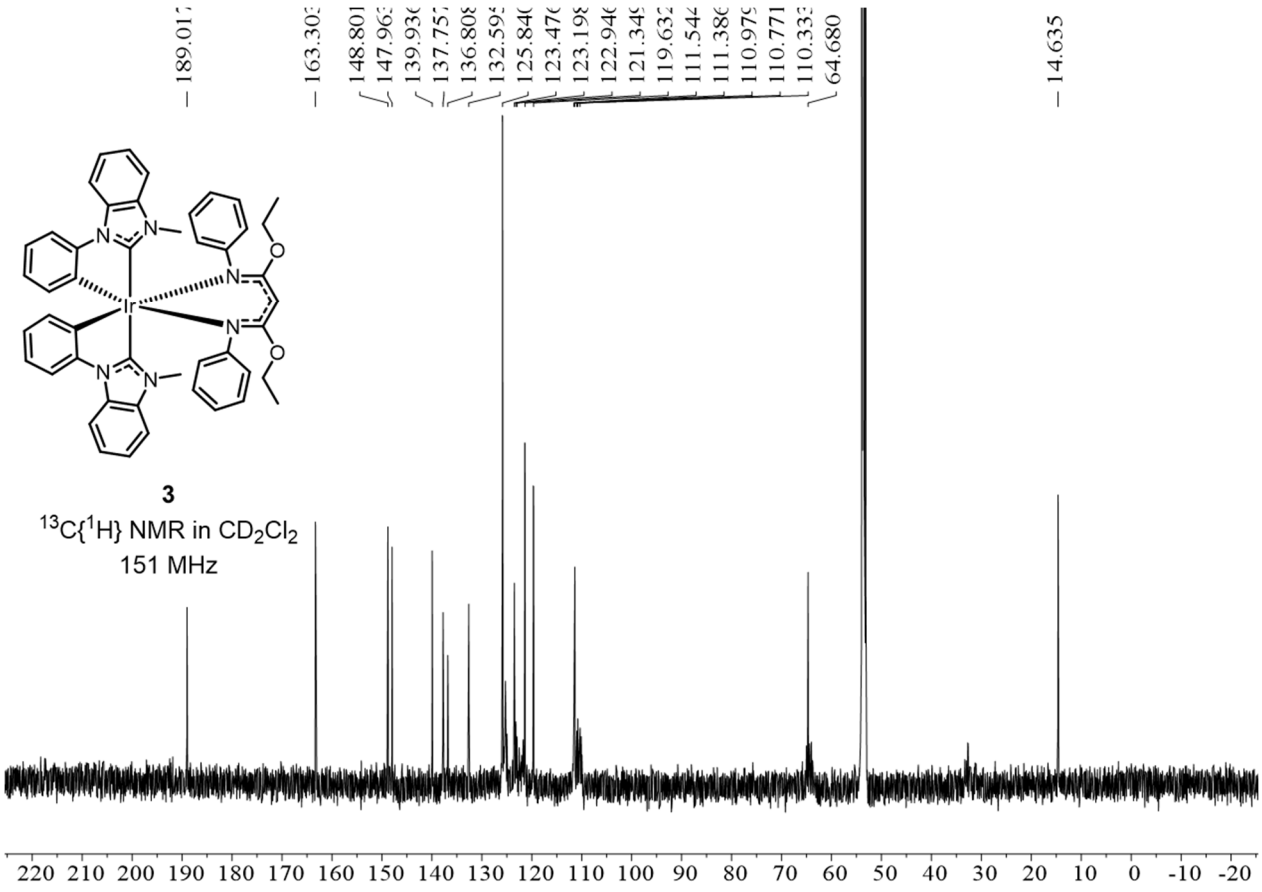


Fig. S6. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(pmb)_2(NacNac^{OEt})$ (**3**), recorded at 151 MHz in CD_2Cl_2.

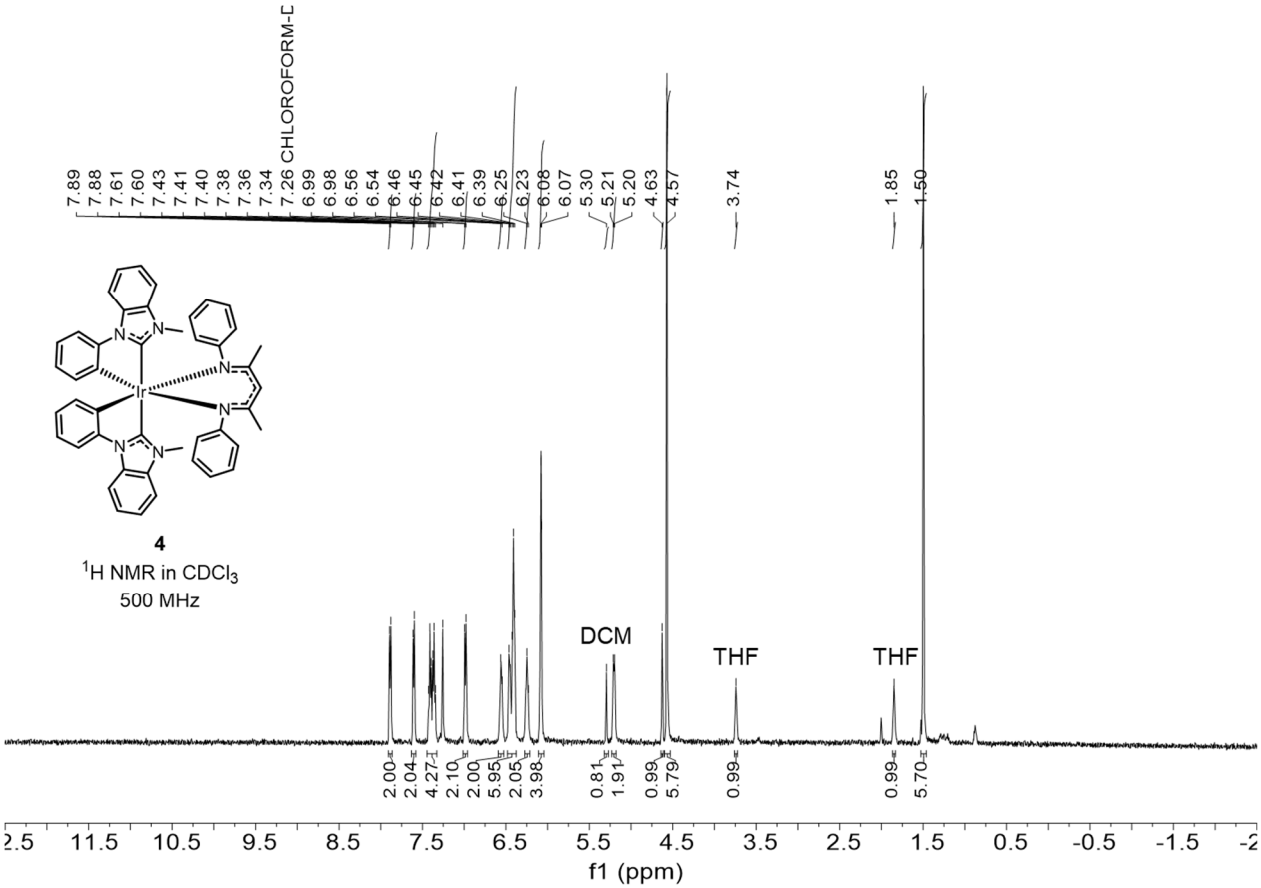


Fig. S7. ^{1}H NMR spectrum of Ir(pmb)$_2$(NacNac^{Me}) (**4**), recorded at 500 MHz in $CDCl_3$.

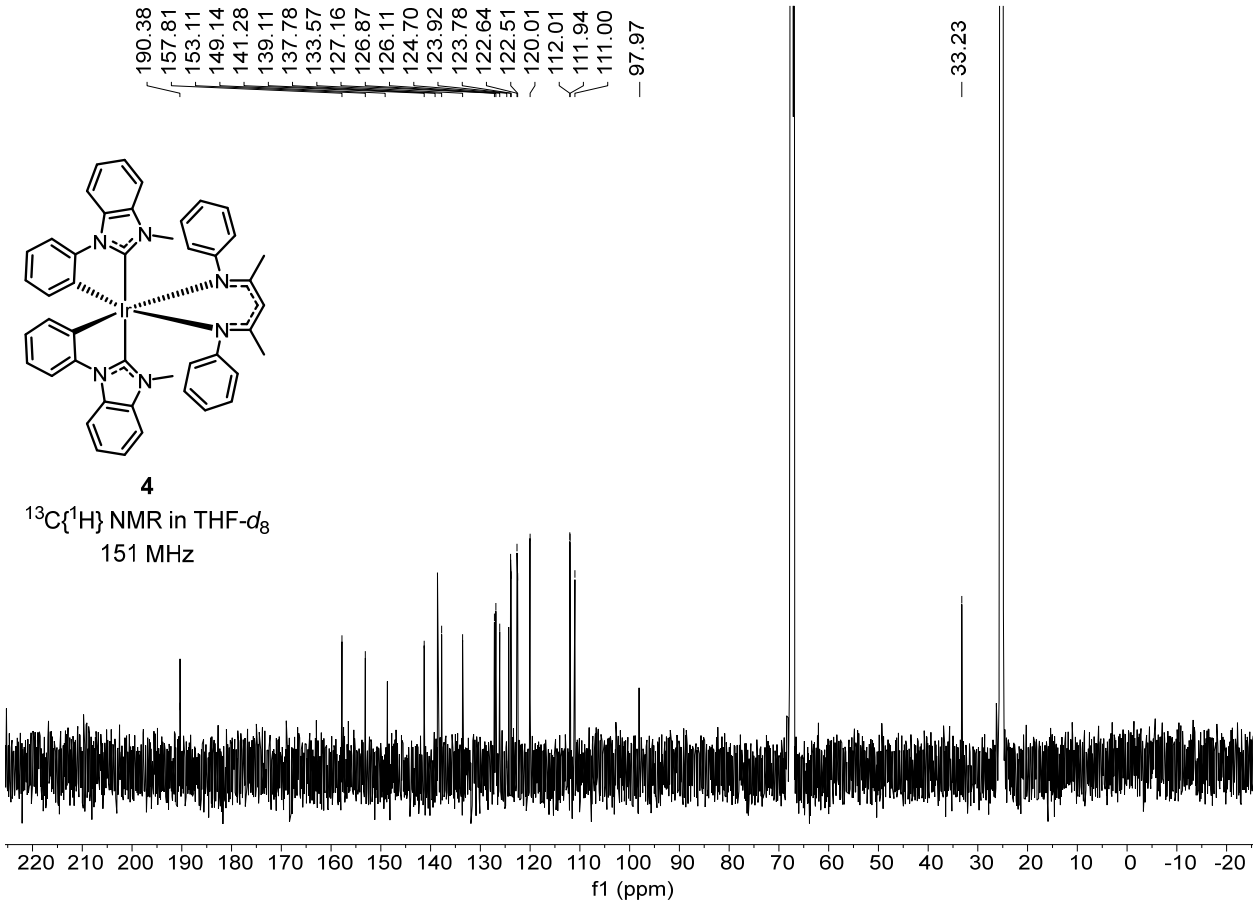


Fig. S8. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(pmb)_2(NacNac^{Me})$ (**4**), recorded at 151 MHz in THF-d_8.

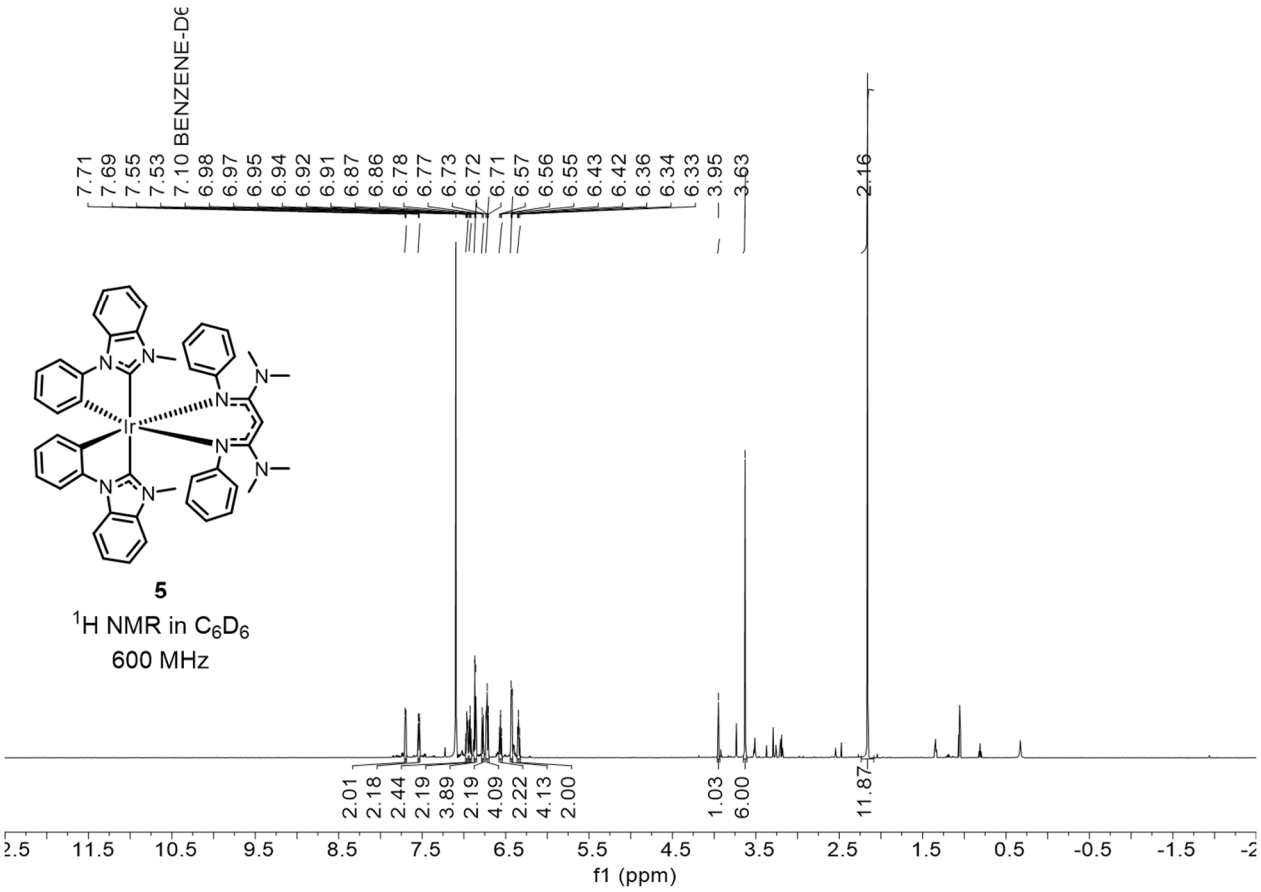


Fig. S9. ^{1}H NMR spectrum of Ir(pmb)$_2$(NacNac^{NMe2}) (**5**), recorded at 600 MHz in C_6D_6.

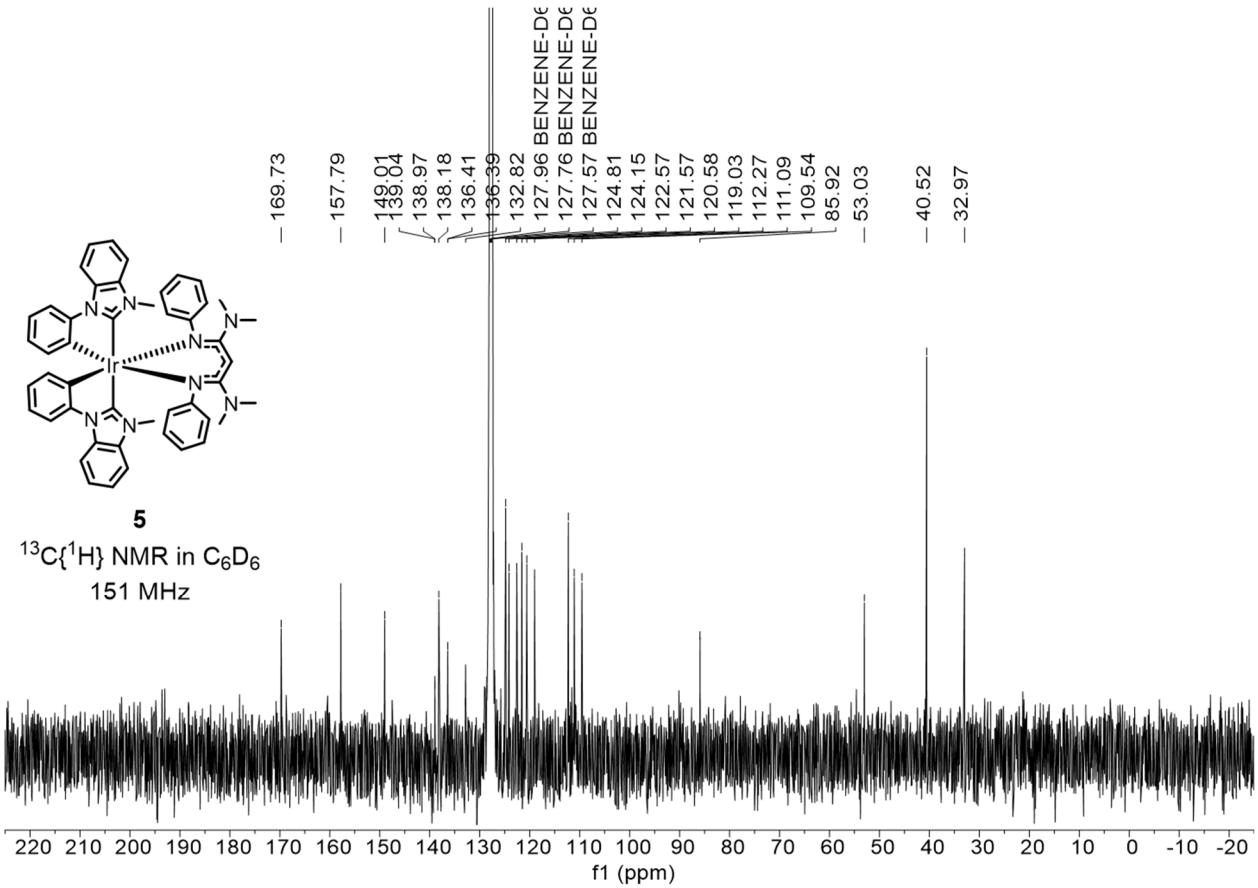


Fig. S10. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(pmb)_2(NacNac^{NMe2})$ (**5**), recorded at 151 MHz in C_6D_6.

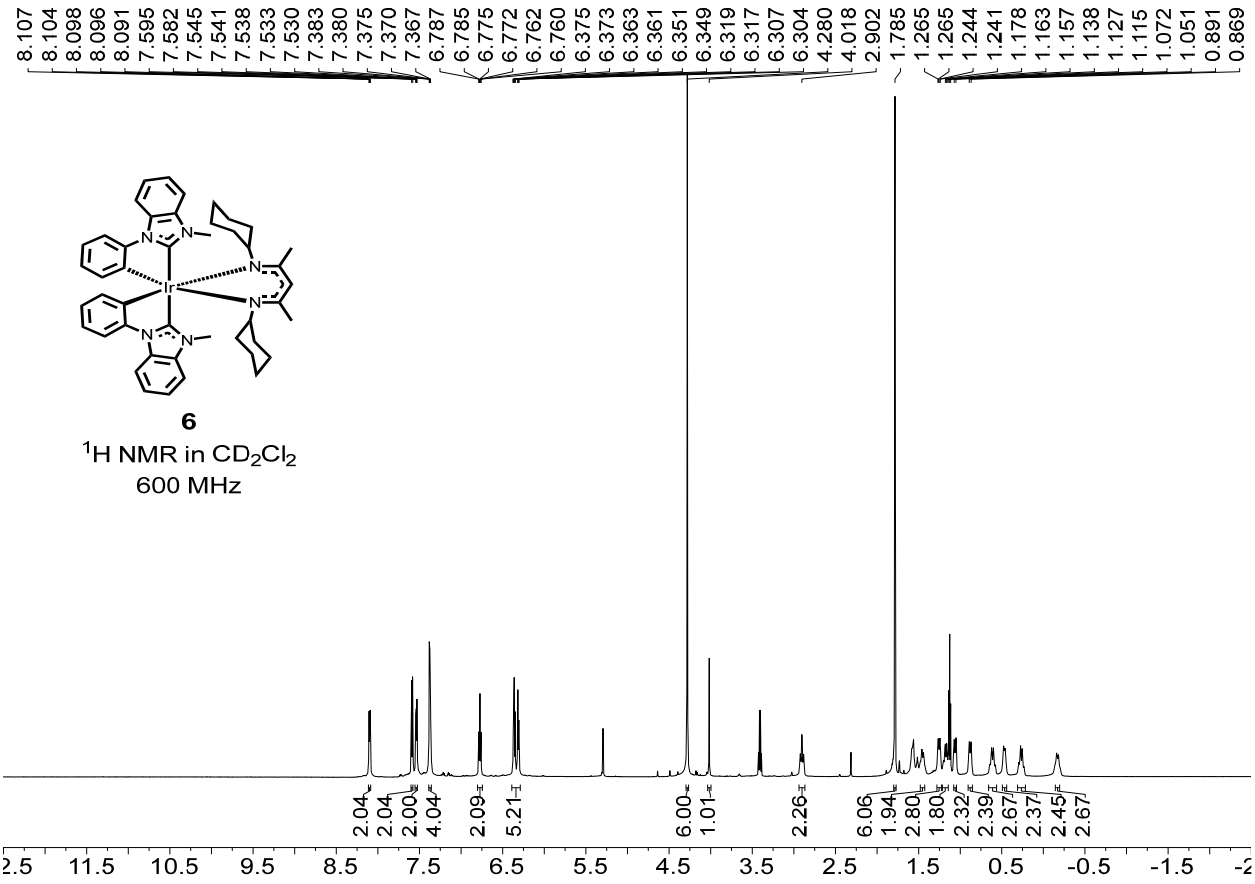


Fig. S11. ^{1}H NMR spectrum of Ir(pmb)$_2$(NacNac^{Cy}) (**6**), recorded at 600 MHz in CD_2Cl_2.

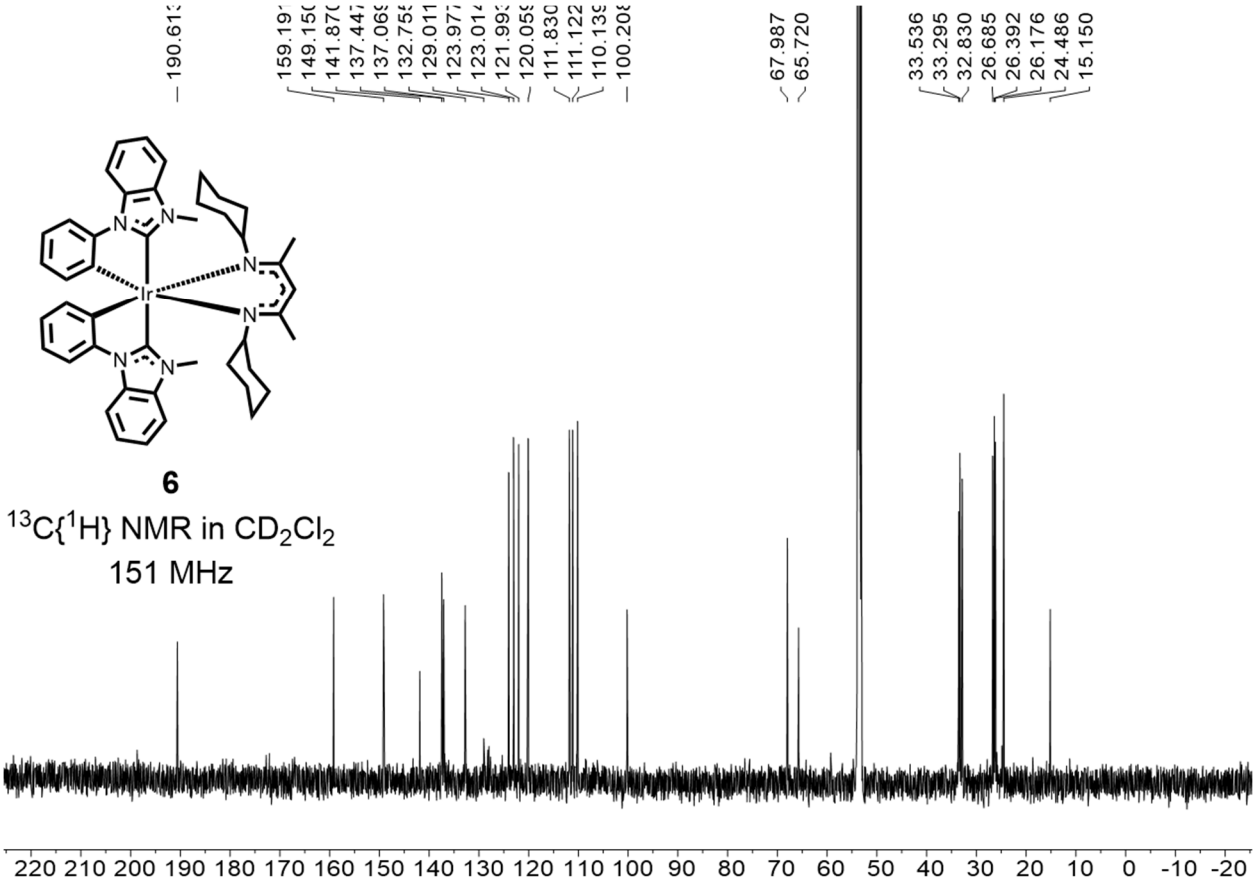


Fig. S12. $^{13}C\{^{1}H\}$ NMR spectrum of $Ir(pmb)_2(NacNac^{Cy})$ (**6**), recorded at 151 MHz in CD_2Cl_2.

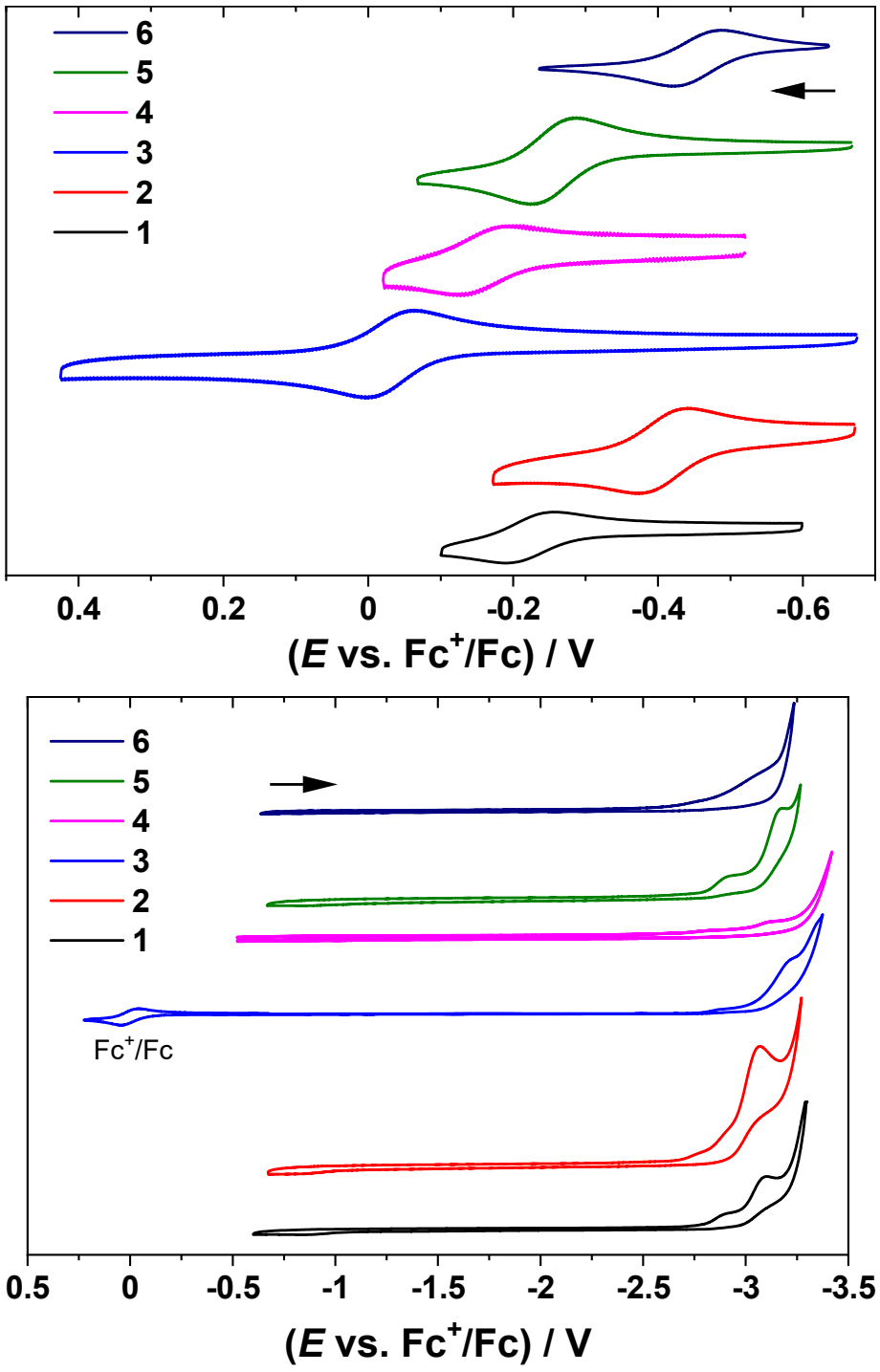


Fig. S13. Overlaid cyclic voltammograms of complexes **1**–**3**, **5**, and **6**, recorded in CH_3CN, and **4** recorded in propylene carbonate, with a scan rate of 0.1 V/s. All solutions included 0.1 M $TBAPF_6$ electrolyte and measurements were made at room temperature. A glassy carbon working electrode, platinum wire counter electrode, and silver wire pseudoreference electrode were used. Potentials are referenced to an internal standard of ferrocene.

Table S2. Summary of the differences in peak potentials (ΔE_p) and peak current ratios ($i_{p,c}$ / $i_{p,a}$) for the Ir^{IV}/Ir^{III} couples shown in the top panel of Figure S13. All measurements were conducted with a scan rate of 0.1 V/s.

Compound	ΔE_p / mV	$i_{p,c}$ / $i_{p,a}$
1	66	0.36
2	67	0.84
3	64	0.93
4	67	0.45
5	64	0.77
6	63	1.0

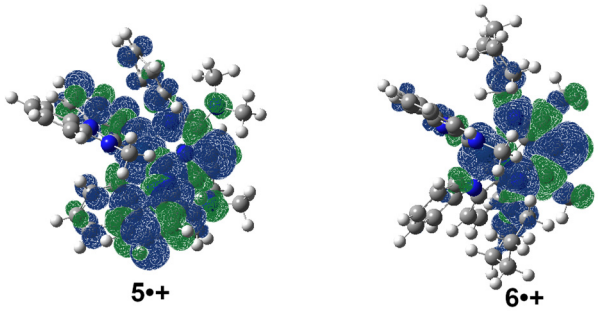


Figure S14. Spin-density plots for the radical cations of complexes **5** and **6**, shown at an isovalue of 0.004 au. The orientation of the molecules places the NacNac ancillary ligand on the right side of the structure.

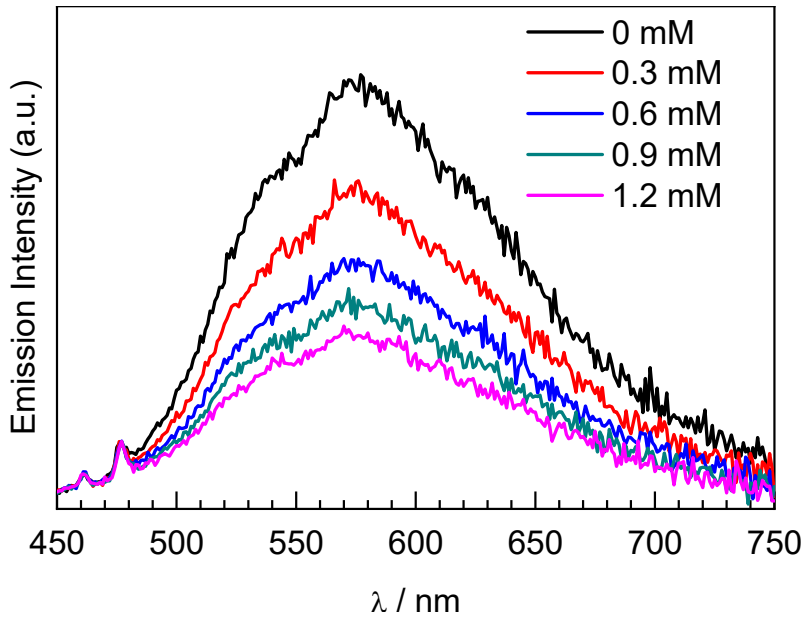
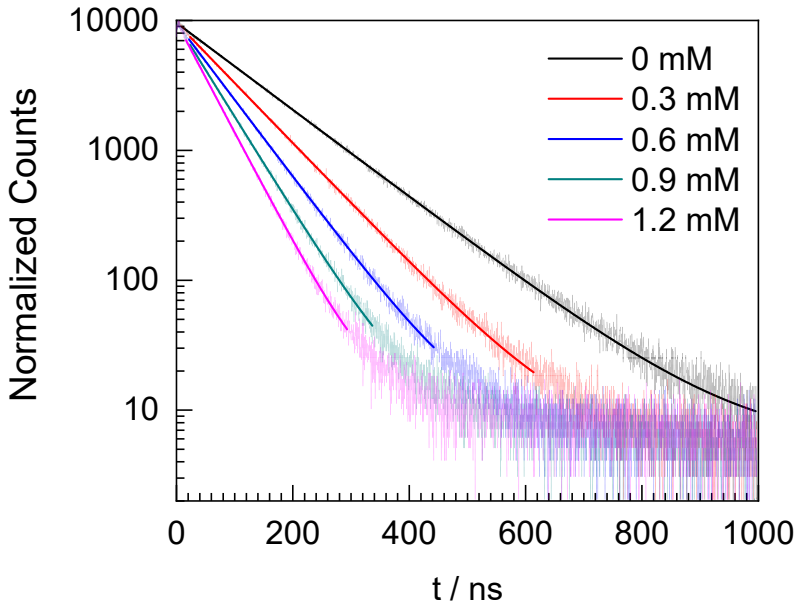
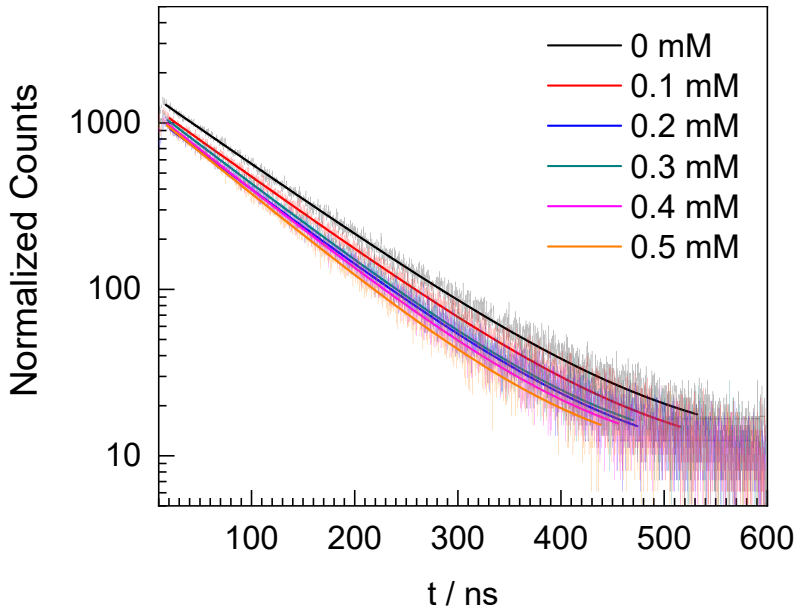


Figure S15. Steady-state photoluminescence quenching for complex **1** in the presence of increasing concentrations of benzophenone (indicated in the legend). The data was recorded in acetonitrile at room temperature.



[BP] / mM	τ / ns
0	129
0.30	94
0.60	73
0.90	60
1.2	51

Figure S16. Time-resolved photoluminescence quenching for complex **1** in the presence of increasing concentrations of benzophenone (indicated in the legend). Both the raw data and the fitted decay curbes are shown. The data was recorded in acetonitrile at room temperature.



[AP] / mM	τ / ns
0	100
0.15	97
0.30	93
0.45	91
0.60	88
0.75	85

Figure S17. Time-resolved photoluminescence quenching for complex **1** in the presence of increasing concentrations of acetophenone (indicated in the legend). Both the raw data and the fitted decay curbes are shown. The data was recorded in acetonitrile at room temperature.

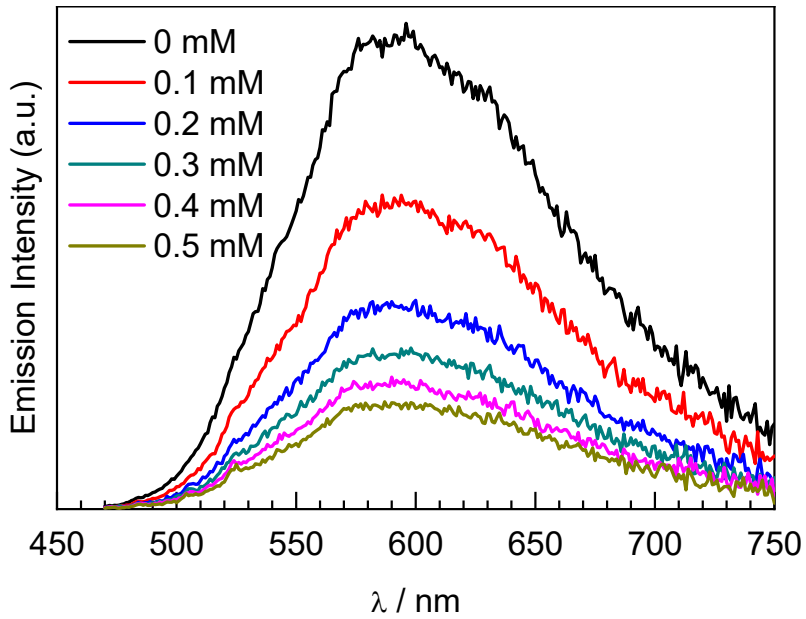
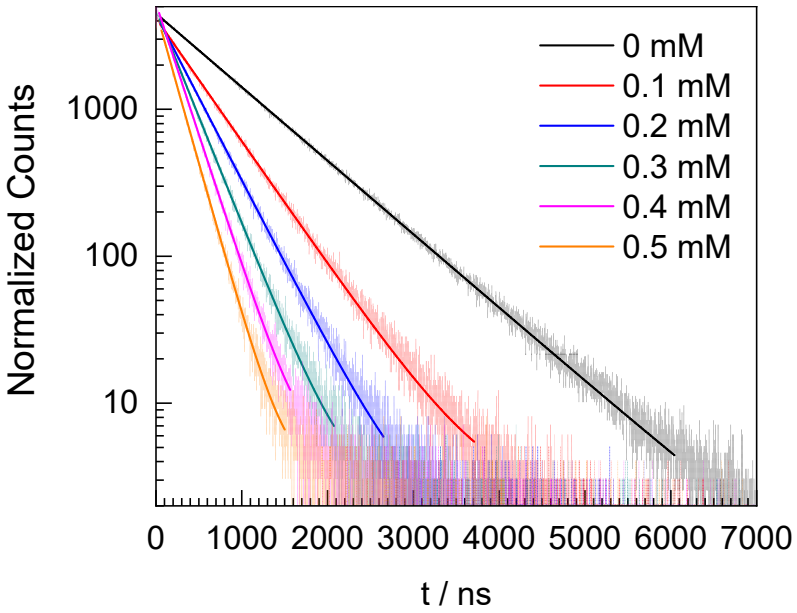
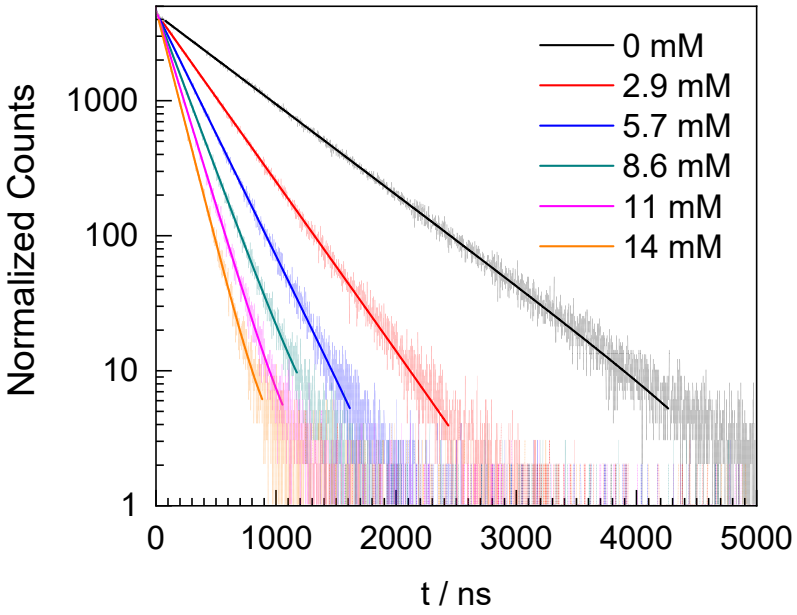


Figure S18. Steady-state photoluminescence quenching for complex **5** in the presence of increasing concentrations of benzophenone (indicated in the legend). The data was recorded in acetonitrile at room temperature.



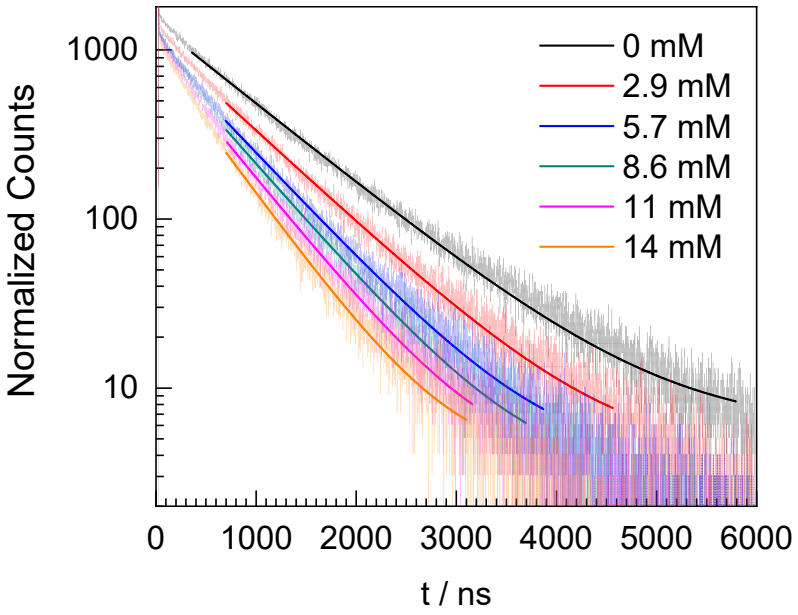
[BP] / mM	τ / ns
0	867
0.10	518
0.20	384
0.30	298
0.40	242
0.50	209

Figure S19. Time-resolved photoluminescence quenching for complex **5** in the presence of increasing concentrations of benzophenone (indicated in the legend). Both the raw data and the fitted decay curbes are shown. The data was recorded in acetonitrile at room temperature.



[AP] / mM	τ / ns
0	648
2.9	347
5.7	240
8.6	183
11	149
14	125

Figure S20. Time-resolved photoluminescence quenching for complex **5** in the presence of increasing concentrations of acetophenone (indicated in the legend). The data was recorded in acetonitrile at room temperature.



[AP] / mM	τ / ns
0	944
2.9	792
5.7	691
8.6	643
11	595
14	536

Figure S21. Time-resolved photoluminescence quenching for complex **7** in the presence of increasing concentrations of acetophenone (indicated in the legend). The data was recorded in acetonitrile at room temperature.

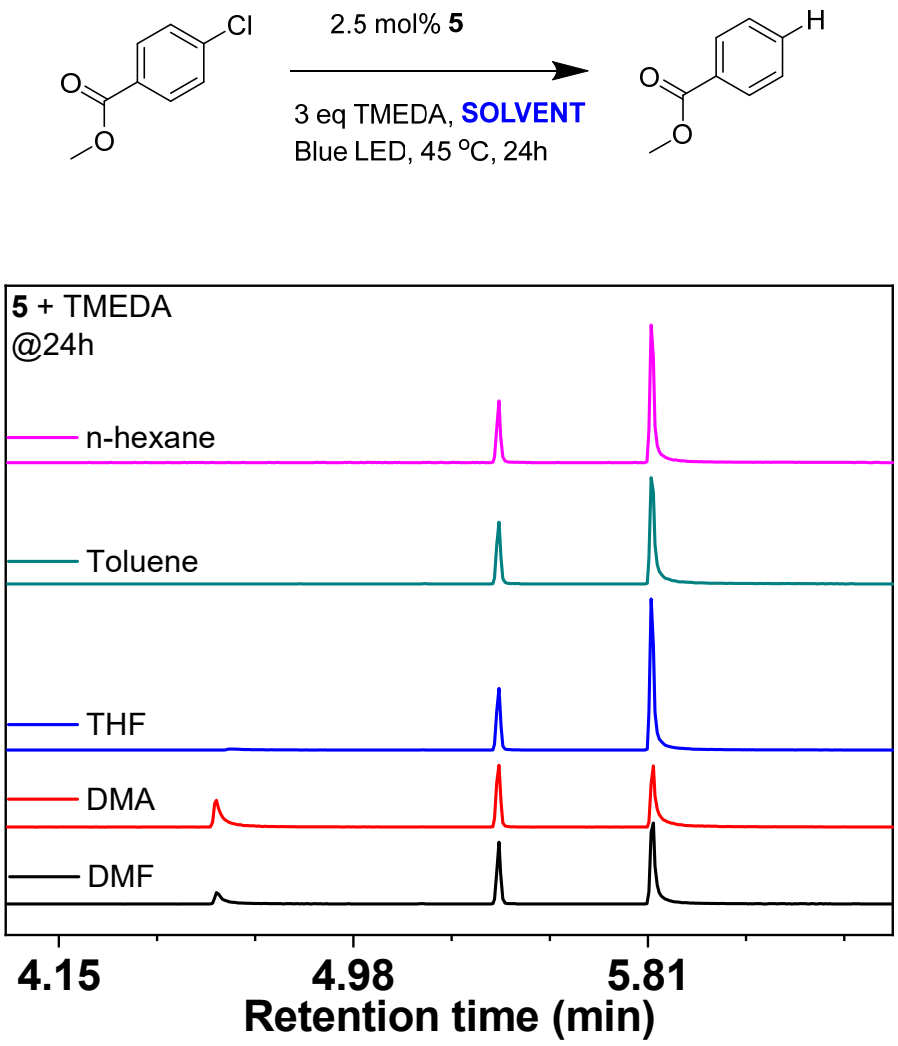


Fig. S22. Solvent optimization for the photocatalytic hydrodehalogenation with complex **5**.

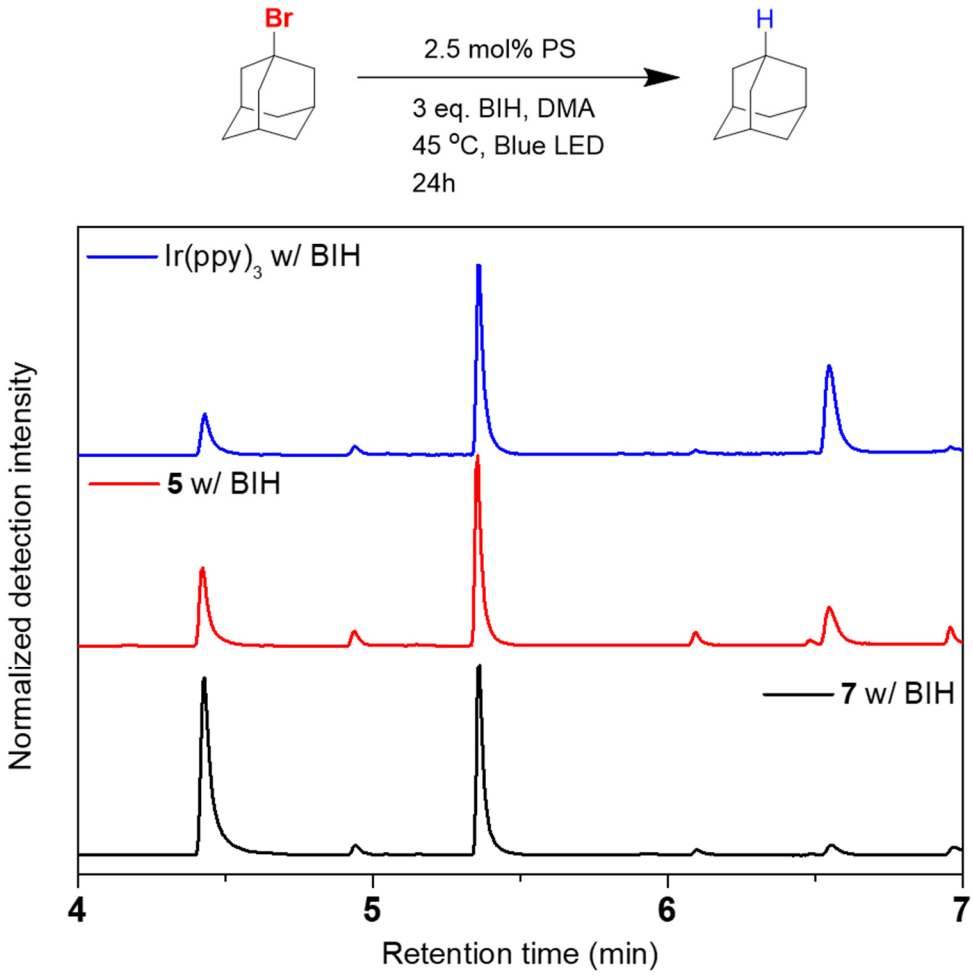


Fig. S23. Photocatalytic hydrodehalogenation of 1-bromoadamantane with complexes **7**, **5**, and $Ir(ppy)_3$ (**10**).

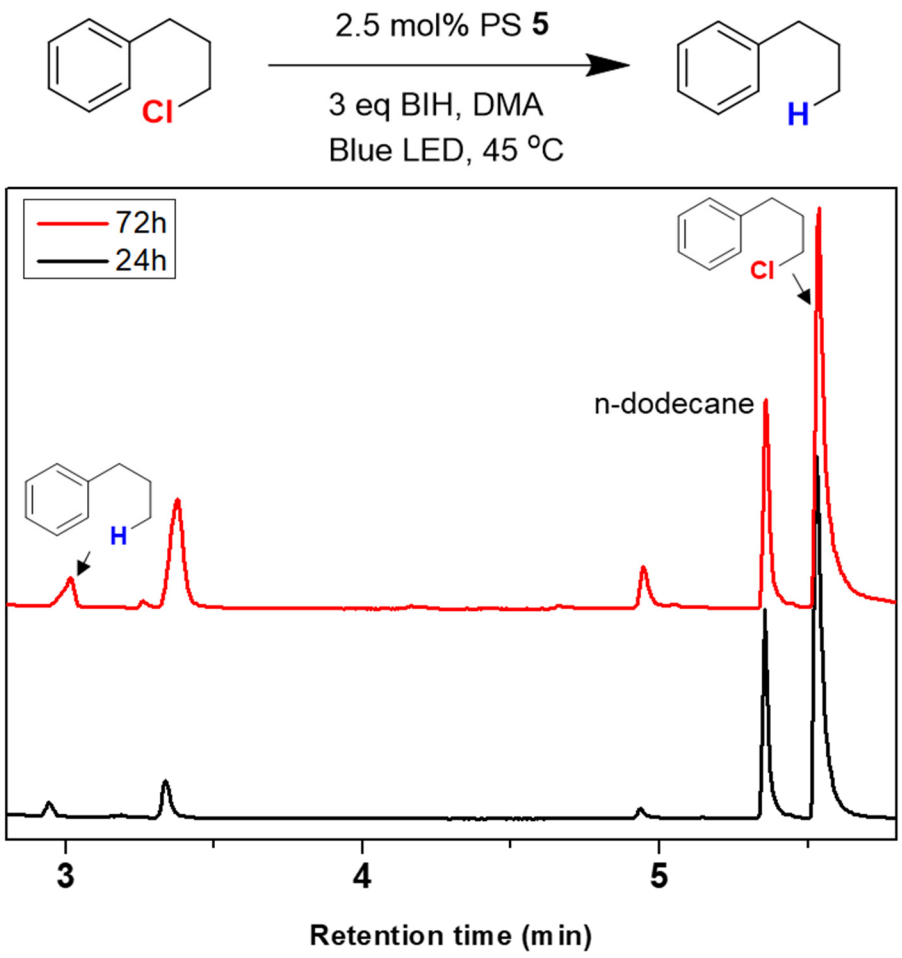


Fig. S24. Photocatalytic hydrodehalogenation of 3-(chloropropyl)benzene with complex **5**.

Table S3. Calculated atomic coordinates (Å) of **5**.

C	10.497293	9.950667	9.971570
N	11.582168	10.118302	9.157396
C	12.728221	9.562795	9.723938
C	12.336818	8.973798	10.945871
N	10.963036	9.211255	11.054400
C	14.039710	9.526918	9.274820
C	14.979739	8.880992	10.075424
C	14.602393	8.292903	11.288029
C	13.283135	8.330067	11.738143
H	14.323838	9.987427	8.336159
H	16.014517	8.835677	9.755951
H	15.350756	7.796232	11.895202
H	13.022981	7.868558	12.678448
C	11.533961	10.720314	7.830756
H	10.484447	10.780396	7.541650
H	12.077399	10.080133	7.127475
H	11.965009	11.725109	7.839931
C	8.635774	8.935746	11.434649
C	7.592997	8.261874	12.088857
C	7.833733	7.407464	13.167749
C	9.132778	7.203903	13.625424
C	10.201509	7.817444	12.971587
C	9.947567	8.642095	11.880714
H	6.572097	8.417779	11.753052
H	7.002843	6.905618	13.654376
H	9.323799	6.557336	14.474953
H	11.209566	7.632528	13.316390
C	6.484721	10.353855	9.922144
N	5.450900	11.177219	10.255570
C	4.223874	10.604099	9.929221
C	2.930530	11.074440	10.099433
C	1.885649	10.266730	9.657375
C	2.143903	9.025839	9.063244
C	3.444866	8.554678	8.893361
C	4.495933	9.355277	9.333544
N	5.888438	9.235403	9.336481
H	2.742139	12.035151	10.562792
H	0.861734	10.601581	9.777487
H	1.315182	8.412048	8.728445
H	3.610116	7.592085	8.434525
C	5.590590	12.544775	10.751767
H	6.633589	12.827892	10.634237
H	5.316001	12.607641	11.808206

H	4.963340	13.201272	10.141187
C	8.131607	8.737880	8.744322
C	9.050423	7.927409	8.060288
C	8.651706	6.773557	7.379433
C	7.314786	6.387400	7.377923
C	6.367748	7.167357	8.042789
C	6.774567	8.324558	8.697055
H	10.103622	8.192427	8.072763
H	9.391206	6.169104	6.862600
H	7.001677	5.483533	6.866859
H	5.333078	6.854492	8.043209
Ir	8.513732	10.335374	9.957174
N	8.550911	11.981829	8.540005
N	8.914003	11.960290	11.347159
C	9.524329	12.915786	8.617668
C	10.360509	13.072641	9.743265
H	11.345361	13.491296	9.573358
C	10.006773	12.721490	11.052772
C	7.403706	12.240056	7.733191
C	6.818811	11.203506	6.993554
C	6.795129	13.506167	7.711546
C	5.653423	11.423224	6.265924
H	7.280702	10.222388	7.016987
C	5.635676	13.723098	6.970778
H	7.234294	14.313716	8.288584
C	5.053535	12.683038	6.246452
H	5.211148	10.601564	5.711342
H	5.177831	14.707784	6.970177
H	4.143982	12.850243	5.680285
C	8.140182	12.337751	12.474376
C	7.967537	13.698431	12.806689
C	7.442204	11.386657	13.231218
C	7.123769	14.082671	13.842087
H	8.485044	14.453621	12.224102
C	6.590449	11.779297	14.260970
H	7.572437	10.338925	13.001351
C	6.418794	13.126651	14.576850
H	7.002325	15.138037	14.067642
H	6.062593	11.017076	14.826291
H	5.755755	13.427562	15.380467
N	9.793420	13.713966	7.517746
C	10.389726	15.039579	7.652885
H	11.436213	15.057145	7.314546
H	9.820839	15.760003	7.048132
H	10.346982	15.345737	8.700780

C	9.491840	13.311270	6.145142
H	8.594345	13.812154	5.759512
H	10.350931	13.560184	5.507015
H	9.318437	12.234306	6.106627
N	10.799063	13.153030	12.092564
C	10.854783	12.424273	13.362178
H	11.902400	12.354157	13.681342
H	10.262243	12.919080	14.142048
H	10.461765	11.416802	13.210907
C	11.705542	14.288792	11.965387
H	11.746130	14.820313	12.924131
H	12.726066	13.981067	11.693932
H	11.327160	14.976181	11.203117

Table S4. Calculated atomic coordinates (Å) of **6**.

C	10.419643	9.662768	10.094060
N	11.569117	9.830289	9.408595
C	12.541225	8.947178	9.845099
C	11.966210	8.174586	10.861845
N	10.662616	8.642031	10.982989
C	13.851526	8.777940	9.430077
C	14.596716	7.796393	10.067297
C	14.036234	7.020910	11.082260
C	12.721538	7.193801	11.496304
H	14.277446	9.388037	8.642864
H	15.626676	7.631686	9.773387
H	14.638994	6.261106	11.566076
H	12.331478	6.573041	12.287711
C	11.797763	10.776590	8.342439
H	12.118749	10.248435	7.442174
H	12.569266	11.492254	8.632300
H	10.867226	11.298826	8.151049
C	8.410307	8.999933	11.584024
C	7.307023	8.647421	12.364956
C	7.358288	7.627900	13.312162
C	8.532709	6.916647	13.501801
C	9.655741	7.228647	12.743541
C	9.580297	8.249969	11.806501
H	6.373955	9.188024	12.239286
H	6.477121	7.390892	13.900152
H	8.586329	6.118764	14.234053
H	10.562779	6.664437	12.899407
C	6.495434	10.724139	10.071667
N	5.637398	11.700385	10.425647
C	4.335117	11.349953	10.112848
C	3.149122	12.040260	10.297981
C	1.983261	11.424716	9.865508
C	2.019334	10.164173	9.269205
C	3.210998	9.474525	9.084100
C	4.383979	10.082419	9.517582
N	5.729926	9.732048	9.510110
H	3.132602	13.019977	10.759814
H	1.033208	11.930150	9.992966
H	1.094738	9.705110	8.938947
H	3.193664	8.501854	8.617186
C	6.005928	12.990090	10.959705
H	7.087801	13.013191	11.058399
H	5.538539	13.144580	11.934106

H	5.678435	13.779186	10.279388
C	7.837233	8.816039	8.964824
C	8.580505	7.818430	8.331504
C	7.981814	6.732817	7.695914
C	6.601712	6.603371	7.692661
C	5.818289	7.574576	8.307200
C	6.436405	8.658566	8.913700
H	9.663948	7.883494	8.328039
H	8.599067	5.983218	7.210700
H	6.125326	5.754124	7.215780
H	4.744613	7.458531	8.308275
Ir	8.505352	10.392128	10.087714
N	8.598638	11.807194	8.393084
N	9.135749	12.020923	11.457561
C	9.301132	13.940786	7.320441
H	9.279404	13.458334	6.348431
H	10.235408	14.497549	7.402484
H	8.488235	14.671007	7.353437
C	9.193280	12.975613	8.486249
C	9.817420	13.474357	9.646705
H	10.352536	14.402020	9.485398
C	9.739662	13.096671	11.002228
C	10.391784	14.119790	11.914134
H	9.662657	14.868795	12.233842
H	11.174997	14.643970	11.366455
H	10.836361	13.684883	12.804216
C	7.853483	11.401175	7.189695
H	7.310032	10.510918	7.505095
C	6.758485	12.356210	6.702002
H	6.139695	12.657735	7.553717
H	7.173023	13.269529	6.271759
C	5.904128	11.669339	5.639480
H	5.130007	12.356049	5.282514
H	5.382423	10.813146	6.085890
C	6.760363	11.183335	4.475798
H	7.210864	12.049813	3.974566
H	6.137385	10.679370	3.729957
C	7.864082	10.249324	4.957489
H	8.490444	9.932986	4.117332
H	7.408400	9.339381	5.367972
C	8.728033	10.900032	6.035178
H	9.443818	10.173066	6.428849
H	9.311921	11.710555	5.587937
C	9.017151	11.738411	12.898600
H	8.309565	10.909600	12.939066

C	10.299355	11.192971	13.539775
H	10.728010	10.427189	12.890997
H	11.053411	11.980506	13.639789
C	9.999579	10.611360	14.918545
H	9.345294	9.739210	14.798509
H	10.923395	10.249192	15.381500
C	9.319969	11.632839	15.822782
H	10.020729	12.450621	16.035504
H	9.067785	11.178701	16.786545
C	8.070807	12.208117	15.165484
H	7.617592	12.967361	15.811001
H	7.325192	11.411816	15.046191
C	8.391971	12.812632	13.799822
H	7.482043	13.205484	13.339828
H	9.062878	13.659883	13.951986

Table S5. Calculated atomic coordinates (Å) of $\mathbf{5}^{+}$.

C	10.489548	9.961525	10.040155
N	11.578077	10.184984	9.285808
C	12.697922	9.609993	9.868421
C	12.269885	8.969616	11.036334
N	10.897124	9.196940	11.096434
C	14.021804	9.609921	9.461090
C	14.930141	8.948126	10.272363
C	14.516602	8.317547	11.446995
C	13.188948	8.317801	11.850890
H	14.336150	10.111767	8.554360
H	15.976965	8.926366	9.993787
H	15.250141	7.816679	12.067726
H	12.914367	7.833972	12.775514
C	11.608028	10.810201	7.981408
H	10.585781	10.943395	7.642189
H	12.134255	10.154571	7.286143
H	12.115862	11.774258	8.022528
C	8.571323	8.964132	11.460277
C	7.519447	8.304762	12.095328
C	7.734429	7.379535	13.111985
C	9.026259	7.085456	13.518598
C	10.104582	7.696911	12.891373
C	9.867304	8.604403	11.868878
H	6.497396	8.524953	11.807249
H	6.888881	6.893132	13.586351
H	9.206520	6.373462	14.315752
H	11.106126	7.439602	13.200193
C	6.417706	10.419456	9.932219
N	5.398447	11.214701	10.299823
C	4.182713	10.619525	9.999835
C	2.888991	11.063504	10.218332
C	1.858813	10.229715	9.812112
C	2.127755	8.997316	9.214993
C	3.425443	8.557118	8.994930
C	4.464419	9.393218	9.389287
N	5.853526	9.314656	9.350539
H	2.689717	12.016117	10.693322
H	0.831232	10.536223	9.967450
H	1.303680	8.359805	8.916961
H	3.587595	7.589588	8.545874
C	5.491948	12.568291	10.800239
H	6.513316	12.911921	10.684308
H	5.204973	12.616842	11.851045

H	4.833131	13.206767	10.210864
C	8.089031	8.798216	8.787495
C	9.003964	7.990362	8.113217
C	8.601699	6.883695	7.371311
C	7.258629	6.549602	7.300429
C	6.314270	7.324651	7.964057
C	6.734764	8.426776	8.692582
H	10.061878	8.222725	8.157847
H	9.341234	6.282012	6.853839
H	6.933540	5.687973	6.728635
H	5.271742	7.057028	7.888193
Ir	8.476829	10.401399	9.992948
N	8.500620	11.990533	8.492463
N	8.882322	12.006417	11.350582
C	9.351721	13.012537	8.593687
C	10.199314	13.191574	9.727250
H	11.082389	13.785390	9.546683
C	10.015690	12.725976	11.021325
C	7.420133	12.093062	7.576205
C	7.150064	11.065612	6.674355
C	6.576072	13.206481	7.599632
C	6.058565	11.146270	5.821218
H	7.806171	10.205075	6.642884
C	5.485151	13.281267	6.747298
H	6.778671	14.014958	8.292980
C	5.218072	12.251277	5.853133
H	5.867417	10.337779	5.123821
H	4.837568	14.150654	6.785742
H	4.364671	12.311283	5.187314
C	8.195623	12.423142	12.491984
C	8.196354	13.776129	12.882951
C	7.421968	11.522295	13.232032
C	7.453163	14.195367	13.969863
H	8.758064	14.502537	12.307580
C	6.694674	11.949266	14.330679
H	7.413906	10.482091	12.943762
C	6.700056	13.286057	14.707826
H	7.454368	15.245565	14.240094
H	6.114308	11.227362	14.894828
H	6.123502	13.619055	15.563013
N	9.535117	13.899093	7.574428
C	10.044086	15.234179	7.811913
H	11.126816	15.298860	7.649788
H	9.556185	15.922123	7.117069
H	9.815087	15.557345	8.825783

C	9.426887	13.541846	6.174392
H	8.522480	13.949845	5.712567
H	10.299176	13.941995	5.650111
H	9.420839	12.461991	6.050335
N	10.925156	12.996916	11.984853
C	11.015350	12.230287	13.212598
H	12.062275	11.974475	13.389041
H	10.641200	12.797744	14.070555
H	10.446618	11.307387	13.130387
C	11.969244	13.979559	11.777219
H	12.389978	14.244418	12.746233
H	12.776993	13.595920	11.143817
H	11.563897	14.887031	11.326345

Table S6. Calculated atomic coordinates (Å) of $\mathbf{6}^{+}$.

C	10.465126	9.624899	10.051030
N	11.620580	9.778544	9.378670
C	12.593672	8.926801	9.878410
C	12.001220	8.186148	10.906126
N	10.686029	8.636421	10.969760
C	13.919481	8.764204	9.510271
C	14.658495	7.826843	10.214126
C	14.081238	7.089710	11.249483
C	12.752950	7.254301	11.614645
H	14.363300	9.349466	8.714567
H	15.700080	7.668887	9.960974
H	14.684483	6.369577	11.789650
H	12.352212	6.673329	12.430455
C	11.862476	10.644837	8.246334
H	12.389804	10.083435	7.474536
H	12.463010	11.507692	8.538216
H	10.910054	10.974120	7.850095
C	8.422924	9.000438	11.530544
C	7.308992	8.671518	12.302060
C	7.336075	7.642689	13.240107
C	8.491571	6.901286	13.421961
C	9.627476	7.200803	12.679141
C	9.581455	8.241003	11.762642
H	6.385837	9.227726	12.179517
H	6.447874	7.420235	13.822034
H	8.521203	6.088434	14.138485
H	10.517846	6.608279	12.822246
C	6.511822	10.642179	10.041459
N	5.620581	11.550798	10.470903
C	4.326523	11.117662	10.228127
C	3.110909	11.718719	10.510038
C	1.966882	11.029945	10.139090
C	2.050951	9.786061	9.511264
C	3.270676	9.187483	9.229004
C	4.423844	9.873159	9.595195
N	5.788879	9.619466	9.491529
H	3.055974	12.682123	11.001656
H	0.994253	11.461828	10.342554
H	1.140248	9.267408	9.235800
H	3.288773	8.221518	8.748924
C	5.930707	12.840436	11.040473
H	7.001824	12.997407	10.961459
H	5.622996	12.880775	12.086555

H	5.411356	13.621909	10.483698
C	7.921275	8.812962	8.879512
C	8.702907	7.880692	8.199295
C	8.141555	6.801641	7.521520
C	6.767832	6.621155	7.519792
C	5.950383	7.529566	8.181537
C	6.529731	8.603195	8.841389
H	9.781837	7.989540	8.188181
H	8.783712	6.099830	6.999916
H	6.321265	5.779458	7.002986
H	4.881728	7.379688	8.168155
Ir	8.546249	10.393614	10.024275
N	8.645746	11.808303	8.394662
N	9.219239	11.983915	11.372518
C	9.556099	13.858391	7.277243
H	9.288992	13.452064	6.310214
H	10.600856	14.171348	7.238649
H	8.958388	14.756892	7.452241
C	9.380624	12.892964	8.423995
C	10.113064	13.286692	9.573979
H	10.781111	14.120327	9.391380
C	10.001151	12.949607	10.944074
C	10.819055	13.859800	11.828256
H	10.289823	14.799743	12.003286
H	11.748794	14.104423	11.313171
H	11.070669	13.421405	12.786311
C	7.789793	11.495396	7.230392
H	7.193473	10.648811	7.565032
C	6.773051	12.575799	6.854720
H	6.231835	12.889346	7.752428
H	7.249360	13.466214	6.442763
C	5.803602	12.015184	5.817307
H	5.088757	12.791342	5.529437
H	5.220306	11.200665	6.264295
C	6.545700	11.492626	4.593079
H	7.053924	12.327871	4.095078
H	5.836414	11.080779	3.869134
C	7.571707	10.434304	4.979337
H	8.120050	10.091822	4.097091
H	7.052014	9.558099	5.385805
C	8.559826	10.953251	6.021332
H	9.211369	10.140654	6.353144
H	9.199212	11.713913	5.566683
C	8.935473	11.811808	12.813060
H	8.098777	11.111449	12.822903

C	10.060695	11.118214	13.592979
H	10.411410	10.247767	13.040186
H	10.917821	11.785050	13.718693
C	9.544997	10.699251	14.966923
H	8.768000	9.937226	14.835692
H	10.355120	10.228494	15.531707
C	8.975410	11.881133	15.742146
H	9.785695	12.580768	15.982564
H	8.560747	11.541958	16.696087
C	7.910643	12.613819	14.934523
H	7.552267	13.489663	15.483168
H	7.043992	11.957545	14.788150
C	8.454286	13.051880	13.576561
H	7.684210	13.578947	13.010657
H	9.264618	13.761533	13.746296