SUPPORTING INFORMATION

Cyclometalated *N*-heterocyclic carbene iridium(III) complexes with naphthalimide chromophores: A novel class of phosphorescent heteroleptic compounds

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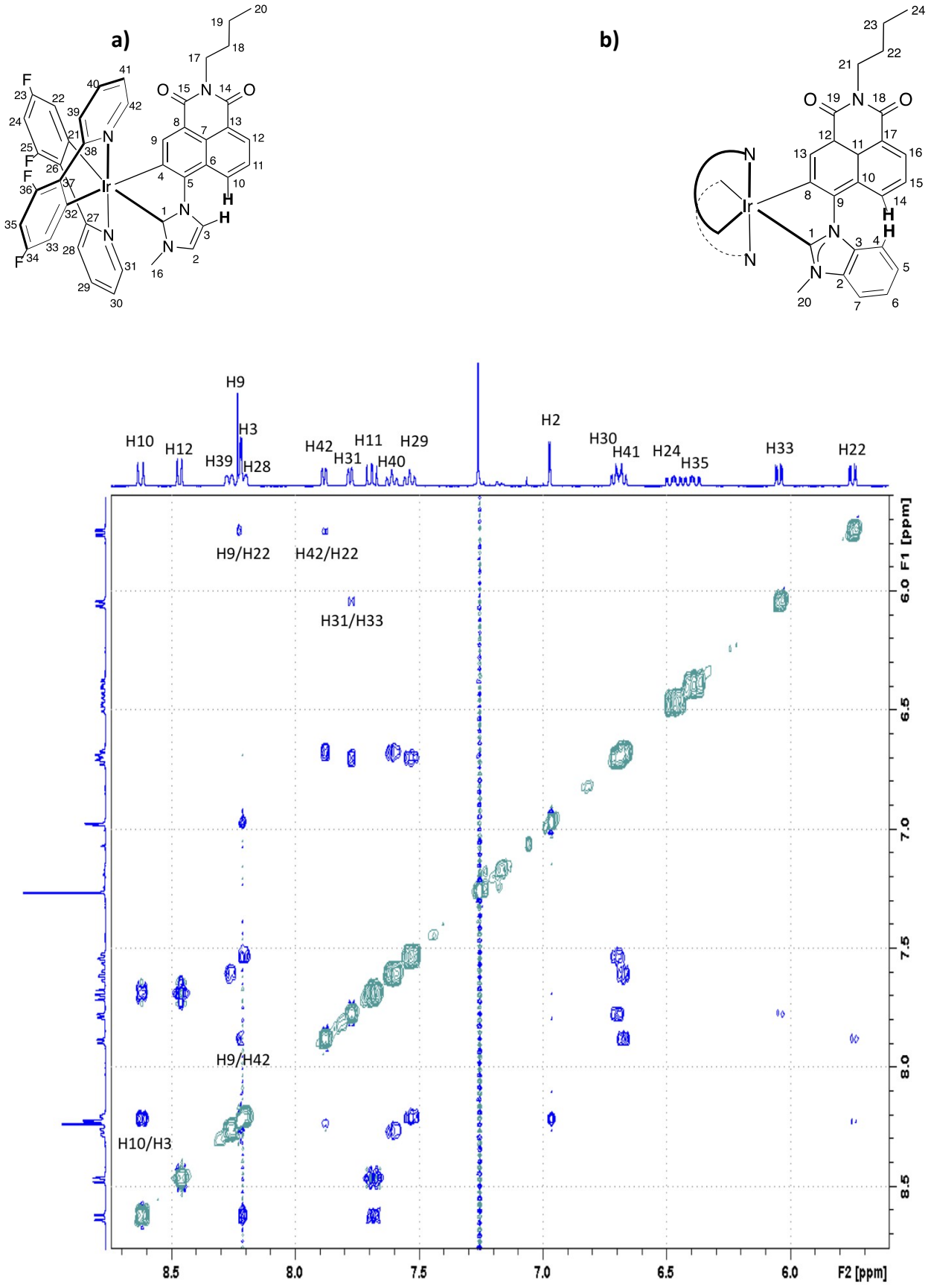


Figure S1. a) ^{1}H-^{1}H correlation for complex **4a** *via* 2D NOESY experiments. b) Numbering of molecule **5b** showing only the correlation between H4 and H14.

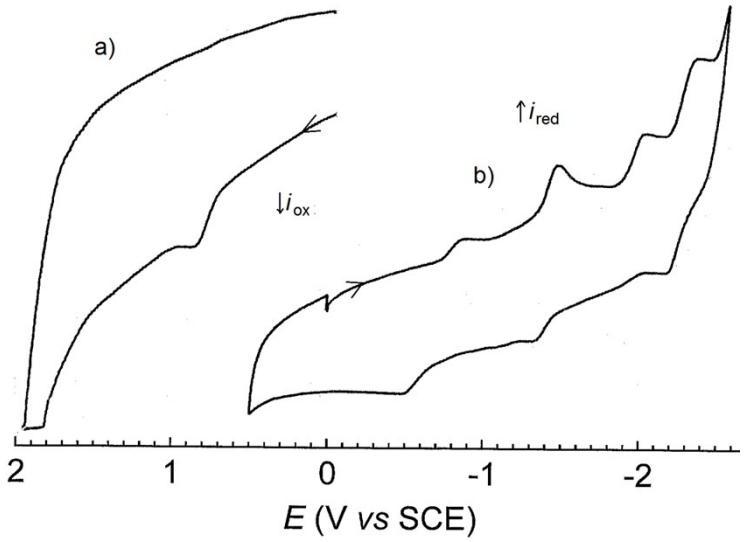


Figure S2. Cyclic voltammetry of complex **3a** (1 mM) in acetonitrile containing nBu$_4$NBF$_4$ (0.2 M) at a vitreous carbon disk electrode (d = 1 mm) with a scan rate of 0.5 Vs^{-1}: a) Oxidation first; b) Reduction first.

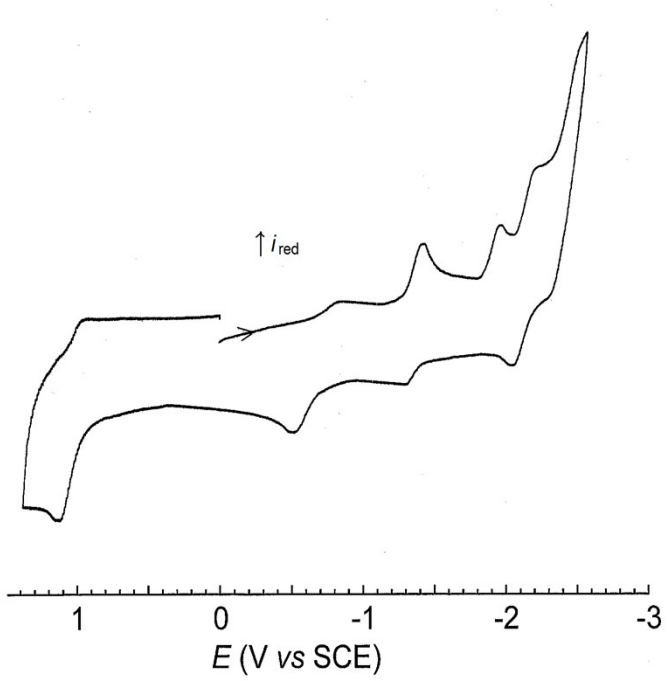


Figure S3. Cyclic voltammetry of complex **4a** (0.5 mM) in acetonitrile containing nBu$_4$NBF$_4$ (0.2 M) at a vitreous carbon disk electrode (d = 1 mm) with a scan rate of 0.5 Vs^{-1}: Reduction first.

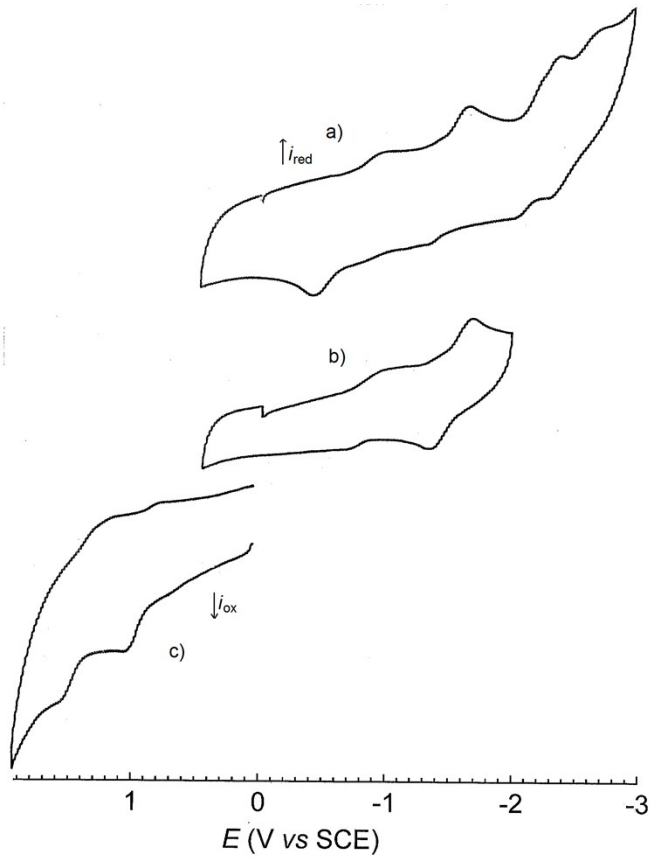


Figure S4. Cyclic voltammetry of complex **5a** (2 mM) in acetonitrile containing nBu$_4$NBF$_4$ (0.2 M) at a vitreous carbon disk electrode (d = 1 mm) with a scan rate of 1 Vs^{-1}: a) Reduction first; b) Reduction first; c) Oxidation first.

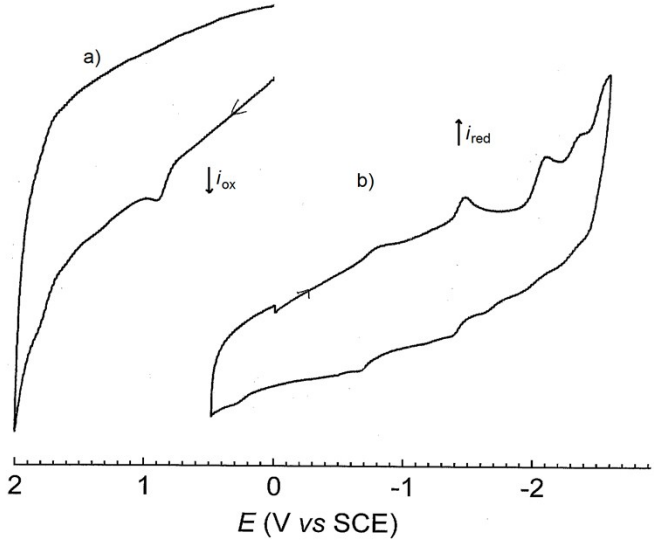


Figure S5. Cyclic voltammetry of complex **3b** (1 mM) in acetonitrile containing nBu$_4$NBF$_4$ (0.2 M) at a vitreous carbon disk electrode (d = 1 mm) with a scan rate of 0.5 Vs^{-1}: a) Oxidation first; b) Reduction first.

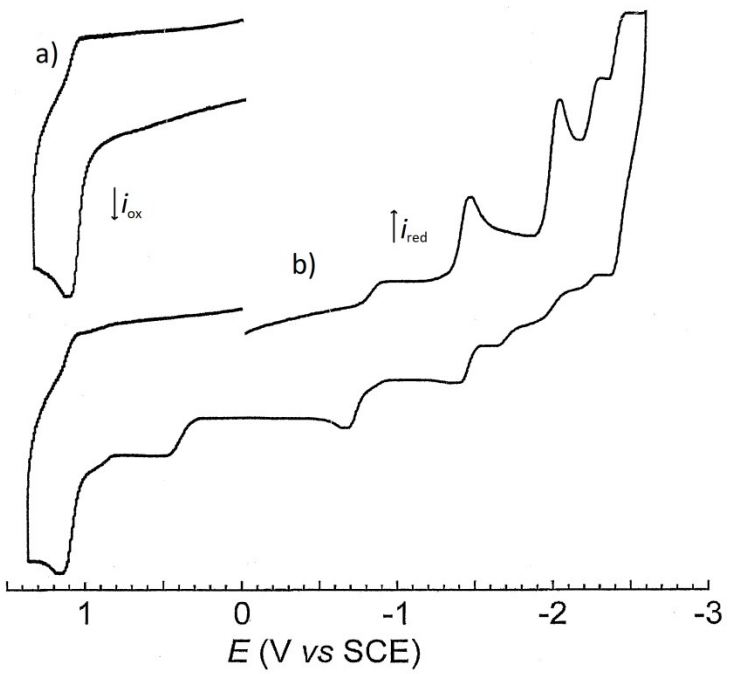


Figure S6. Cyclic voltammetry of complex **4b** (0.5 mM) in acetonitrile containing nBu$_4$NBF$_4$ (0.2 M) at a vitreous carbon disk electrode (d = 1 mm) with a scan rate of 0.5 Vs^{-1}: a) Reduction first; b) Oxidation first; c) Reduction first

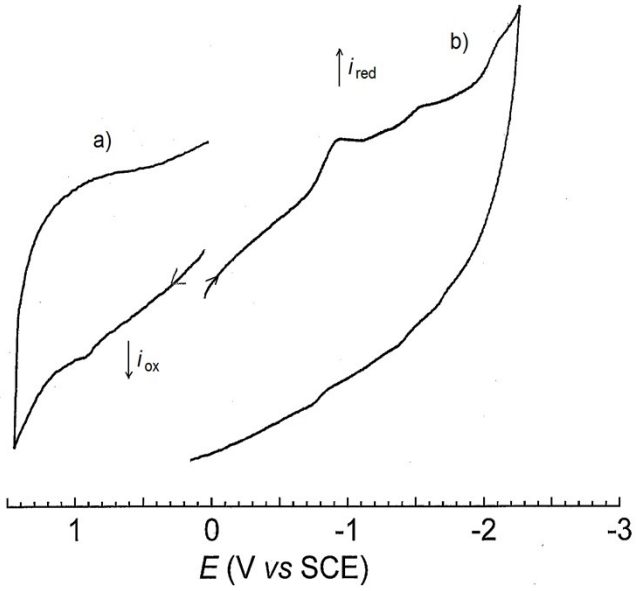


Figure S7. Cyclic voltammetry of complex **5b** (< 0.5 mM due to poor solubility) in acetonitrile containing nBu$_4$NBF$_4$ (0.2 M) at a vitreous carbon disk electrode (d = 1 mm) with a scan rate of 0.5 Vs^{-1}: a) Oxidation first; b) Reduction first.

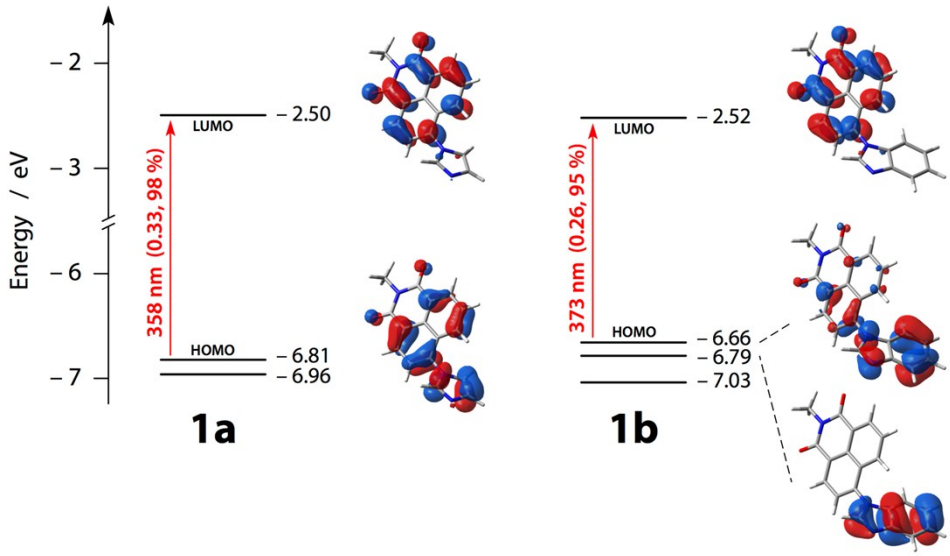


Figure S8. Energy diagram showing the energy of frontier molecular orbitals of proligands **1a** and **1b** (in eV) obtained at the PCM-M06/6-31G(d,p) level of theory, in dichloromethane. The Kohn–Sham molecular orbitals involved in the $S_0 \rightarrow S_1$ transitions are also reported for clarity (isovalue: 0.04 $e^{1/2}$ $bohr^{-3/2}$), together with the wavelength associated with such transition, its oscillator strength and the percentage of the orbital contribution.

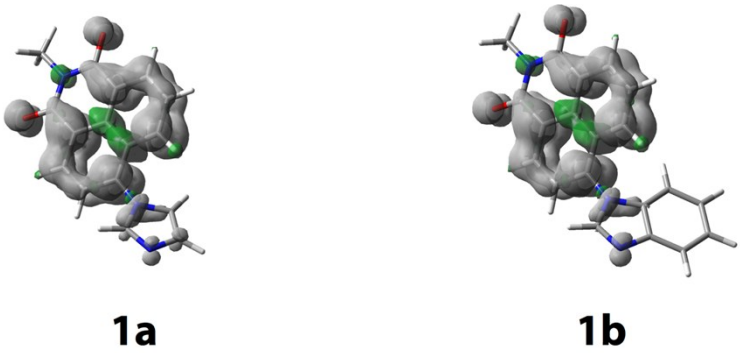


Figure S9. Spin-density distribution for the lowest-energy triplet state (T_1) of proligands **1a** and **1b**, computed at the PCM-M06/6-31G(d,p) level of theory, in dichloromethane; isovalue: 0.002 e $bohr^{-3}$.

Table S1. Crystal data for complexes **2a**, **4a**, **5a** and **5b**.

Compound	**2a**	**4a**	**5a**	**5b**
Empirical formula	C20 H21 I N3 O2.50	C42 H30 F4 Ir N5 O2	C46 H34 Ir N5 O2	C50 H36 Ir N5 O2
Formula weight	470.30	904.91	880.98	931.04
Temperature	200(1) K	200(1) K	200(1) K	200(1) K
Wavelength	0.71073 Å	1.54178 Å	1.54178 Å	1.54178 Å
Crystal system	Trigonal	Triclinic	Triclinic	Triclinic
Space group	R -3 c :H	P -1	P -1	P -1
Unit cell dimensions	a = 14.9781(5) Å	a = 14.8872(7) Å	a = 13.5805(3) Å	a = 9.3652(4) Å
	b = 14.9781(5) Å	b = 16.5821(7) Å	b = 16.1341(4) Å	b = 12.4098(5) Å
	c = 96.166(3) Å	c = 18.9038(8) Å	c = 21.2216(5) Å	c = 16.8233(7) Å
	α = 90°	α = 93.720(3)°	α = 74.302(1)°	α = 99.293(2)°
	β = 90°	β = 104.970(3)°	β = 89.578(1)°	β = 98.218(2)°
	γ = 120°	γ = 96.521(3)°	γ = 65.159(1)°	γ = 90.072(2)°
Volume	18683.8(14) $Å^3$	4457.4(3) $Å^3$	4032.1(2) $Å^3$	1909.14(14) $Å^3$
Z	36	4	4	2
Density (calculated)	1.505 $g.cm^{-3}$	1.348 $g.cm^{-3}$	1.451 $g.cm^{-3}$	1.620 $g.cm^{-3}$
Absorption coefficient	1.563 mm^{-1}	6.251 mm^{-1}	6.749 mm^{-1}	7.165 mm^{-1}
F(000)	8460	1784	1752	928
Crystal size	0.5 x 0.25 x 0.02 mm^3	0.30 x 0.10 x 0.05 mm^3	0.4 x 0.1 x 0.05 mm^3	0.17 x 0.12 x 0.03 mm^3
θ range for data collection	1.626° to 30.539°	3.101° to 66.689°	3.159° to 66.710°	3.610° to 66.607°
Index ranges	-19<=h<=18	-17<=h<=17	-16<=h<=16	-11<=h<=11
	-21<=k<=21	-19<=k<=19	-18<=k<=19	-14<=k<=14
	-137<=l<=137	-19<=l<=22	-25<=l<=25	-20<=l<=17
Reflections collected	57852	79873	56906	26772
Independent reflections	6366 [R(int) = 0.0501]	15721 [R(int) = 0.0442]	14191 [R(int) = 0.0237]	6729 [R(int) = 0.0267]
Completeness	99.9 %	99.6 %	99.4 %	99.9 %
Absorption correction	Semi-empirical from equivalents			
Max. and min. transmission	1.000 and 0.702	0.891 and 0.386	0.782 and 0.326	0.860 and 0.485
Refinement method	Full-matrix least-squares on F^2			
Data / restraints / parameters	6366 / 0 / 290	15721 / 0 /973	14191 / 25 / 1000	6729 / 0 / 524
Goodness-of-fit on F^2	1.090	1.039	1.035	1.089
Final R indices [I > 2σ(I)]	R1 = 0.0473 wR2 = 0.1331	R1 = 0.0271 wR2 = 0.0659	R1 = 0.0246 wR2 = 0.0611	R1 = 0.0247 wR2 = 0.0637
R indices (all data)	R1 = 0.0710 wR2 = 0.1573	R1 = 0.0374 wR2 = 0.0699	R1 = 0.0265 wR2 = 0.0625	R1 = 0.0259 wR2 = 0.0644
Largest difference peak	1.884 $e.Å^{-3}$	1.213 $e.Å^{-3}$	0.984 $e.Å^{-3}$	2.850 $e.Å^{-3}$
Largest difference hole	-0.988 $e.Å^{-3}$	-0.891 $e.Å^{-3}$	-0.741 $e.Å^{-3}$	-0.464 $e.Å^{-3}$

Table S2. Calculated NTOs couples describing the $S_0 \rightarrow T_1$ transition for all the investigated iridium(III) complexes (**3-5a,b**) in dichloromethane, using PCM at the M06 level of theory. The λ value is the natural transition orbital eigenvalue associated with each NTOs couple.

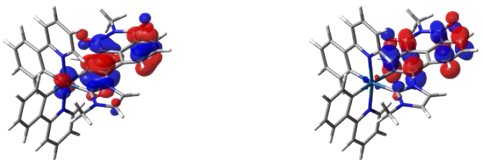
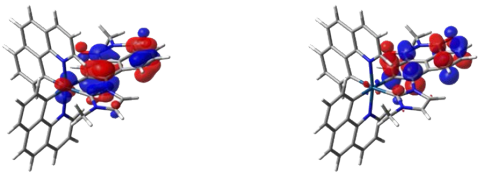
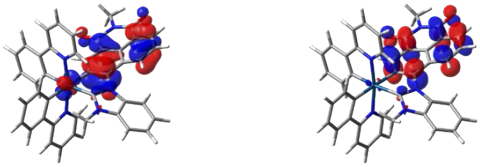
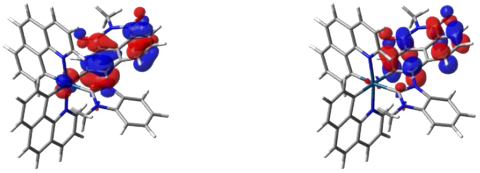
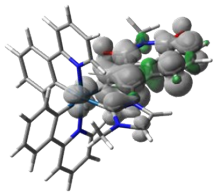
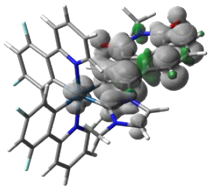
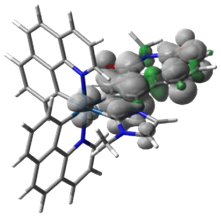
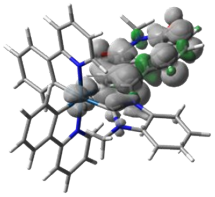
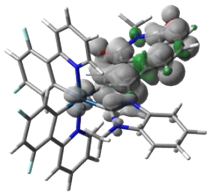
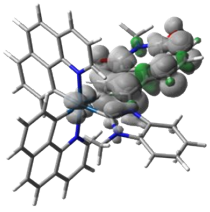
	Transition energy [eV (nm)]	NTO couple hole → electron (λ)	Nature
3a	1.92 (645)	 (98.1%)	^{3}LC on the naphthalimide moiety
4a	1.95 (636)	 (97.8%)	^{3}LC on the naphthalimide moiety
5a	1.92 (647)	 (98.1%)	^{3}LC on the naphthalimide moiety
3b	1.94 (640)	 (98.0%)	^{3}LC on the naphthalimide moiety
4b	1.96 (633)	 (97.7%)	^{3}LC on the naphthalimide moiety
5b	1.94 (640)	 (98.0%)	^{3}LC on the naphthalimide moiety

Table S3. Comparison between the experimentally observed emission in dichlorometane at 298 K and the theoretically computed phosphorescence of all the investigated complexes (**3-5a,b**). The spin-density distribution of the fully optimized emitting state (T_1), computed at the M06 level of theory in dichloromethane, is also reported for clarity; isovalue: 0.002 e bohr^{-3}.

	Exp. emission in DCM at 298 K [nm]	$T_1 - S_0$ adiabatic energy difference [eV (nm)]	T_1 spin-density distribution
3a	670	1.85 (669)	
4a	645	1.90 (656)	
5a	665	1.85 (669)	
3b	690	1.85 (670)	
4b	660	1.89 (657)	
5b	680	1.86 (668)	

DFT optimized geometries

All geometries are calculated at the M06 level of theory using PCM (solvent: dichloromethane). The ECP60MDF pseudopotential, together with the associated correlation-consistent "double-ζ" basis sets, is used for the iridium metal centre, while the 6-31G(d,p) for all other atoms. The geometries of the ground state and the lowest (singlet and/or triplet) excited states are reported in the following sections for proligands **1a,b** and all complexes (**3a,b–5a,b**). All the reported geometries correspond to minima, as verified by frequency calculations.

Proligand 1a

Ground-state (S_0)

C	-1.143284	2.568430	0.130875
C	-1.561132	1.256695	0.052254
C	-0.614218	0.207594	0.009108
C	0.774531	0.514572	0.027083
C	1.166759	1.870636	0.132937
C	0.226738	2.873555	0.181464
H	-1.894415	3.353079	0.165347
C	-1.046135	-1.137286	-0.031770
C	1.692580	-0.573034	-0.028165
H	2.223786	2.117084	0.187670
H	0.544483	3.908748	0.266084
C	1.249376	-1.878003	-0.055637
C	-0.123909	-2.160925	-0.049838
H	1.976205	-2.684045	-0.110652
H	-0.477721	-3.187613	-0.079349
C	-2.484653	-1.458912	-0.051862
O	-2.909334	-2.602520	-0.086383
C	-3.008250	0.967043	0.023197
O	-3.852175	1.847746	0.046148
N	-3.373333	-0.382626	-0.032559
C	-4.791814	-0.722962	-0.064836
H	-5.015108	-1.302624	-0.963932
H	-5.052489	-1.325565	0.809077
N	3.086681	-0.328996	-0.032960
C	4.004081	-0.896070	0.814106
C	3.807522	0.462693	-0.912284
N	5.227211	-0.517048	0.545056
H	3.689644	-1.553895	1.616919
C	5.113180	0.326469	-0.535653
H	3.325085	0.997823	-1.718398
H	5.981474	0.788214	-0.989362
H	-5.361018	0.204693	-0.064152

Lowest singlet excited state (S_1)

C	-1.096639	2.595742	-0.069703
C	-1.546303	1.262457	-0.032568
C	-0.622577	0.194819	-0.019487
C	0.782164	0.489765	-0.044984
C	1.197504	1.834581	-0.091431
C	0.257650	2.870261	-0.099486
H	-1.840309	3.387418	-0.077067
C	-1.065772	-1.152266	0.010594
C	1.651932	-0.627973	-0.028277
H	2.256266	2.079708	-0.138954
H	0.602853	3.900912	-0.132712
C	1.212968	-1.955486	0.003315
C	-0.141308	-2.216797	0.018643
H	1.944119	-2.760606	0.023807
H	-0.521213	-3.233376	0.040176
C	-2.482878	-1.448527	0.030829
O	-2.949667	-2.591897	0.055079
C	-2.975968	0.999168	-0.009242
O	-3.827223	1.892056	-0.014819
N	-3.354311	-0.350086	0.021900
C	-4.773677	-0.668974	0.045225
H	-5.042629	-1.264827	-0.831840
H	-5.014900	-1.254118	0.937161
N	3.073293	-0.384277	-0.023209
C	3.819076	0.054984	1.057180
C	3.931052	-0.541951	-1.028620
N	5.111861	0.190501	0.773903
H	3.349032	0.247654	2.013692
C	5.220041	-0.175357	-0.501557
H	3.633406	-0.874254	-2.012839
H	6.156797	-0.177649	-1.041933
H	-5.327798	0.268220	0.047684

Lowest triplet excited state (T_1)

C	-1.186732	2.614177	0.133945	O	-2.851847	-2.631522	-0.099013
C	-1.585054	1.245213	0.048258	C	-3.015943	0.937636	0.014294
C	-0.623501	0.220333	0.008637	O	-3.870785	1.817791	0.035227
C	0.775479	0.551171	0.043879	N	-3.363129	-0.412719	-0.043446
C	1.131399	1.897784	0.168132	C	-4.775101	-0.775604	-0.080992
C	0.140467	2.920136	0.201042	H	-4.986410	-1.356943	-0.982018
H	-1.960057	3.375206	0.153080	H	-5.028686	-1.384768	0.790599
C	-1.039199	-1.125970	-0.029956	N	3.086675	-0.306634	-0.035761
C	1.702058	-0.530116	-0.002076	C	4.027591	-0.996590	0.698727
H	2.177138	2.176288	0.261132	C	3.798333	0.593038	-0.817626
H	0.461441	3.955094	0.281083	N	5.244645	-0.595906	0.446999
C	1.251367	-1.892632	-0.012281	H	3.732062	-1.749448	1.420808
C	-0.070666	-2.191503	-0.031246	C	5.110758	0.389512	-0.506611
H	1.999854	-2.680159	-0.048119	H	3.307181	1.232566	-1.536775
H	-0.429866	-3.214493	-0.062764	H	5.972696	0.893806	-0.925392
C	-2.455096	-1.468889	-0.058841	H	-5.358594	0.143333	-0.079621

Proligand 1b

Ground-state (S_0)

C	1.749840	2.464863	-0.687218	N	4.197889	-0.139176	0.283795
C	2.271413	1.244578	-0.313044	C	5.625219	-0.307536	0.537690
C	1.426059	0.119705	-0.178127	H	5.778054	-0.702371	1.545136
C	0.030546	0.258573	-0.414546	H	6.051920	-1.014239	-0.178815
C	-0.467884	1.520799	-0.817256	N	-2.180599	-0.822757	-0.481749
C	0.375543	2.599452	-0.947526	C	-2.894804	-1.594577	-1.376604
H	2.423210	3.312104	-0.784695	C	-3.127123	-0.078354	0.216385
C	1.968225	-1.139242	0.165401	N	-4.181216	-1.404448	-1.337005
C	-0.783983	-0.899890	-0.264456	H	-2.368567	-2.269629	-2.044611
H	-1.528077	1.630936	-1.030260	C	-4.363881	-0.458536	-0.339774
H	-0.020690	3.561228	-1.260312	H	6.103171	0.664835	0.435350
C	-0.231846	-2.120785	0.060727	C	-3.022017	0.833666	1.263277
C	1.149700	-2.242355	0.269803	C	-5.546655	0.102021	0.147811
H	-0.882678	-2.984025	0.173145	C	-5.452827	1.019866	1.182499
H	1.589947	-3.200586	0.531239	C	-4.209741	1.377166	1.732931
C	3.415170	-1.287697	0.408137	H	-2.062024	1.104720	1.695898
O	3.932163	-2.352035	0.706402	H	-4.176912	2.094767	2.548986
C	3.723147	1.129655	-0.067648	H	-6.357535	1.471071	1.582654
O	4.480087	2.081344	-0.164317	H	-6.504960	-0.186857	-0.276449

Lowest singlet excited state (S_1)

C	1.732463	2.498579	-0.689296	N	4.175066	-0.134577	0.273382
C	2.267604	1.251565	-0.306146	C	5.600928	-0.301826	0.517422
C	1.422447	0.126843	-0.164713	H	5.763168	-0.701107	1.522435
C	0.011993	0.268830	-0.393990	H	6.026832	-1.008444	-0.200836
C	-0.479591	1.519871	-0.804604	N	-2.177891	-0.879102	-0.391772
C	0.382257	2.618321	-0.945512	C	-2.914485	-1.780804	-1.187498
H	2.409312	3.341937	-0.787525	C	-3.108576	-0.057282	0.186629
C	1.966390	-1.134346	0.167957	N	-4.188999	-1.580737	-1.164894
C	-0.778871	-0.912261	-0.244082	H	-2.387209	-2.530559	-1.767114
H	-1.533908	1.643765	-1.035204	C	-4.360805	-0.502425	-0.298363
H	-0.028896	3.573998	-1.261267	H	6.075740	0.672333	0.413402
C	-0.203299	-2.173114	0.036144	C	-2.991975	0.970855	1.137541
C	1.146434	-2.283760	0.256586	C	-5.525138	0.091154	0.141112
H	-0.854761	-3.038626	0.131460	C	-5.413242	1.137999	1.077127
H	1.608856	-3.233179	0.506153	C	-4.173114	1.560262	1.567517

C	3.397674	-1.282297	0.401171
O	3.922333	-2.357813	0.698086
C	3.698460	1.139826	-0.078241
O	4.473397	2.092776	-0.176865
H	-2.024518	1.290117	1.512685
H	-4.133043	2.362582	2.297333
H	-6.316948	1.623699	1.433211
H	-6.493019	-0.251248	-0.212090

Lowest triplet excited state (T_1)

C	1.740754	2.507655	-0.693952
C	2.270473	1.239626	-0.304035
C	1.427996	0.122988	-0.170377
C	0.018757	0.259248	-0.417974
C	-0.463327	1.503381	-0.836717
C	0.407902	2.622833	-0.960327
H	2.423339	3.347015	-0.777245
C	1.976915	-1.132274	0.163336
C	-0.785508	-0.906795	-0.271384
H	-1.514804	1.620800	-1.083501
H	-0.008478	3.576486	-1.273101
C	-0.195708	-2.179850	0.033804
C	1.136768	-2.298010	0.253725
H	-0.853864	-3.040575	0.124543
H	1.597948	-3.245939	0.510024
C	3.405879	-1.279926	0.404980
O	3.917576	-2.357380	0.701753
C	3.710309	1.129318	-0.061774
O	4.461916	2.094460	-0.159657
N	4.189656	-0.134088	0.287333
C	5.616243	-0.300997	0.540719
H	5.769784	-0.698444	1.547151
H	6.043966	-1.005848	-0.177207
N	-2.177684	-0.861752	-0.438881
C	-2.913380	-1.742868	-1.217473
C	-3.119721	-0.045117	0.191316
N	-4.197537	-1.555628	-1.166858
H	-2.402320	-2.484753	-1.823072
C	-4.364747	-0.499715	-0.281787
H	6.092358	0.672670	0.440346
C	-3.004936	0.968883	1.138326
C	-5.543769	0.089387	0.176208
C	-5.439692	1.111641	1.108016
C	-4.189695	1.539809	1.584252
H	-2.039647	1.301485	1.511771
H	-4.146331	2.337568	2.321444
H	-6.341272	1.588669	1.484172
H	-6.506740	-0.260782	-0.186537

Complex 3a

Ground-state (S_0)

C	5.692661	-2.121878	0.542060
C	5.189016	-0.946950	0.022850
C	3.792898	-0.739869	-0.074552
C	2.890170	-1.774011	0.320143
C	3.451448	-2.937842	0.904298
C	4.813953	-3.108463	1.009409
H	6.769790	-2.247371	0.607961
C	3.289244	0.502322	-0.520418
C	1.499192	-1.507594	0.156391
H	2.805617	-3.695995	1.333444
H	5.208537	-4.009407	1.471588
C	0.979621	-0.250527	-0.163798
C	1.925768	0.737687	-0.510346
H	1.581881	1.731667	-0.799757
C	4.206980	1.565794	-0.948010
O	3.838405	2.656509	-1.358704
C	6.137399	0.098757	-0.406226
O	7.349687	-0.055321	-0.361652
N	5.579223	1.290466	-0.872366
C	6.470560	2.355748	-1.314501
H	6.258681	2.610522	-2.356229
H	6.317852	3.250435	-0.705190
N	0.492099	-2.498330	0.354996
C	0.536315	-3.889395	0.385933
N	-1.544437	-3.182963	0.558211
C	-0.739965	-4.311492	0.528398
H	1.436211	-4.465696	0.250447
H	-1.147530	-5.309802	0.599475
C	-0.805273	-0.629123	-2.889200
C	-0.729295	1.980097	2.169265
C	-0.706012	-0.181497	3.072841
C	-0.856172	2.757698	0.943137
C	-1.217945	2.721429	-1.429642
C	-5.270298	-0.242089	-1.044058
C	-5.369020	0.197599	1.316452
H	-3.502127	0.435701	2.338642
C	-3.470931	-0.591328	-3.455618
C	-1.205178	-0.808636	-4.199452
H	0.243789	-0.630559	-2.603224
C	-0.563809	2.511156	3.452474
C	-0.545747	0.296069	4.359001
H	-0.772762	-1.247577	2.868329
C	-0.749134	4.154642	0.911301
C	-1.110785	4.108326	-1.463317
H	-1.404076	2.188175	-2.364462
C	-6.021422	-0.053033	0.105687
H	-5.779656	-0.433291	-1.988236
H	-5.955934	0.355109	2.220704
C	-2.569178	-0.785615	-4.485674
H	-4.537427	-0.566073	-3.659004
H	-0.460484	-0.959529	-4.974178
C	-0.472622	1.674748	4.549591
H	-0.515916	3.588472	3.580222
H	-0.480590	-0.400389	5.188532
C	-0.873439	4.831725	-0.291940
H	-0.560829	4.719643	1.823578

H	7.494680	2.001379	-1.213226
C	-0.809133	-2.056011	0.420663
Ir	-1.122083	-0.031998	0.070792
C	-3.183198	0.032180	0.238666
N	-1.677865	-0.431450	-1.883615
N	-0.798356	0.627039	2.000611
C	-1.089347	2.000092	-0.232871
C	-3.870026	-0.194825	-0.981393
C	-3.980211	0.244312	1.374672
C	-3.017757	-0.412947	-2.144361
H	-1.211546	4.635958	-2.411027
H	-7.107240	-0.094630	0.062984
H	-2.923200	-0.917818	-5.504599
H	-0.348013	2.090900	5.545703
H	-0.786515	5.915228	-0.322381
C	-2.986310	-3.207090	0.744502
H	-3.253774	-2.723272	1.689048
H	-3.487368	-2.675129	-0.069280
H	-3.319178	-4.246662	0.763009

Lowest triplet excited state (T_1)

C	5.714042	-2.048319	0.642120
C	5.177579	-0.848224	0.095199
C	3.795309	-0.667561	-0.005359
C	2.909769	-1.720671	0.413077
C	3.473335	-2.867500	1.004857
C	4.868396	-3.023662	1.105077
H	6.793912	-2.148387	0.696729
C	3.261132	0.563399	-0.503914
C	1.525876	-1.493076	0.186613
H	2.833270	-3.626437	1.443108
H	5.268418	-3.926916	1.559289
C	0.966096	-0.177972	-0.128232
C	1.872380	0.794487	-0.519817
H	1.527578	1.786905	-0.806254
C	4.160904	1.624932	-0.926000
O	3.778268	2.712506	-1.360700
C	6.104586	0.188805	-0.339383
O	7.327853	0.056900	-0.278213
N	5.532887	1.365039	-0.834287
C	6.414353	2.433178	-1.283149
H	6.205506	2.675644	-2.328847
H	6.248555	3.335090	-0.687131
N	0.545597	-2.491543	0.293602
C	0.626434	-3.881503	0.274199
N	-1.482311	-3.233566	0.380614
C	-0.644941	-4.338153	0.338256
H	1.553259	-4.420735	0.167562
H	-1.028536	-5.348324	0.351689
H	7.441445	2.090149	-1.170740
C	-0.775051	-2.084402	0.333066
Ir	-1.094279	-0.042018	0.093710
C	-3.177388	-0.046594	0.083085
N	-1.493437	-0.341875	-1.933557
N	-0.948882	0.506838	2.077048
C	-1.129921	2.005608	-0.092312
C	-3.755841	-0.226777	-1.194768
C	-4.060296	0.088869	1.164460
C	-2.809081	-0.349330	-2.296244
C	-0.542888	-0.443925	-2.881293
C	-0.955517	1.850358	2.323934
C	-0.907078	-0.362224	3.105294
C	-1.026261	2.696520	1.139549
C	-1.208415	2.785734	-1.253169
C	-5.144708	-0.306708	-1.370223
C	-5.439257	0.011727	0.993661
H	-3.664454	0.241559	2.171152
C	-3.155975	-0.453837	-3.646980
C	-0.836745	-0.552050	-4.226588
H	0.483609	-0.416794	-2.525012
C	-0.911974	2.309940	3.643909
C	-0.866836	0.045184	4.423366
H	-0.910207	-1.415612	2.835354
C	-0.994191	4.096540	1.195197
C	-1.175592	4.176049	-1.199810
H	-1.291238	2.301238	-2.228398
C	-5.986777	-0.194539	-0.274961
H	-5.576180	-0.462280	-2.358116
H	-6.098411	0.108152	1.855373
C	-2.174377	-0.553250	-4.615329
H	-4.204140	-0.444733	-3.930088
H	-0.030599	-0.626894	-4.948819
C	-0.867950	1.413038	4.694790
H	-0.920205	3.378639	3.835427
H	-0.834724	-0.695133	5.215775
C	-1.066421	4.837213	0.025769
H	-0.903861	4.613580	2.149743
H	-1.232236	4.754816	-2.120574
H	-7.064300	-0.261007	-0.404715
H	-2.446463	-0.626986	-5.664714
H	-0.837693	1.772560	5.719684
H	-1.036741	5.923365	0.064326
C	-2.930898	-3.304649	0.495327
H	-3.258803	-2.826048	1.422917
H	-3.408759	-2.795005	-0.346293
H	-3.229319	-4.354431	0.503614

Complex 4a

Ground-state (S_0)

C	6.000676	-2.186995	0.493157
C	5.466797	-1.010546	0.009711
C	4.065470	-0.835839	-0.078273
C	-0.528178	-0.832647	-2.872275
C	-0.502532	1.757688	2.201468
C	-0.443182	-0.422436	3.066939

C	3.189354	-1.902196	0.289648
C	3.781140	-3.068409	0.837939
C	5.147736	-3.208283	0.933397
H	7.080721	-2.287794	0.553132
C	3.531853	0.405922	-0.488215
C	1.791840	-1.664116	0.137310
H	3.157287	-3.854783	1.248016
H	5.565626	-4.112440	1.367909
C	1.244093	-0.412818	-0.155134
C	2.163775	0.608147	-0.474524
H	1.797691	1.601272	-0.738535
C	4.422534	1.505495	-0.882845
O	4.024226	2.598207	-1.258514
C	6.388435	0.071057	-0.388748
O	7.603886	-0.055233	-0.351147
N	5.800563	1.263131	-0.815780
C	6.664649	2.364727	-1.222240
H	6.451782	2.642774	-2.257771
H	6.483249	3.236799	-0.588625
N	0.805271	-2.679053	0.318845
C	0.874994	-4.069077	0.325672
N	-1.217812	-3.404757	0.516091
C	-0.392861	-4.517430	0.464290
H	1.784748	-4.626522	0.178524
H	-0.781443	-5.524225	0.519205
H	7.697651	2.036282	-1.124577
C	-0.503083	-2.263985	0.396667
Ir	-0.858684	-0.243900	0.076709
C	-2.917201	-0.204350	0.249299
N	-1.413670	-0.641432	-1.877426
N	-0.543929	0.404739	2.010341
C	-0.861885	1.787247	-0.212774
C	-3.601413	-0.413585	-0.981935
C	-3.679223	0.000033	1.406262
C	-2.753458	-0.621686	-2.150936
C	-0.638148	2.536712	0.976314
C	-1.002778	2.480082	-1.420728
C	-5.001375	-0.437273	-0.982524
C	-5.060147	-0.035390	1.343823
H	-3.211071	0.176296	2.375320
C	-3.187243	-0.785483	-3.472603
C	-0.909102	-0.999575	-4.189629
H	0.516817	-0.838082	-2.572411
C	-0.360294	2.266583	3.498425
C	-0.304897	0.032283	4.363668
H	-0.484831	-1.485212	2.840968
C	-0.553456	3.930501	0.890434
C	-0.910884	3.860877	-1.442112
H	-1.180149	1.960825	-2.362405
C	-5.754880	-0.258587	0.161793
C	-2.267899	-0.969269	-4.490228
H	-4.246626	-0.759267	-3.690164
H	-0.154305	-1.145163	-4.955396
C	-0.264169	1.407000	4.578184
H	-0.334374	3.338039	3.645480
H	-0.232008	-0.678864	5.179864
C	-0.683593	4.618030	-0.300840
H	-6.838407	-0.284487	0.129000
H	-2.610835	-1.089127	-5.514399
H	-0.158982	1.808385	5.582490
H	-0.609589	5.699244	-0.335262
C	-2.659757	-3.456424	0.695607
H	-2.940875	-2.971876	1.635603
H	-3.165911	-2.942583	-0.126549
H	-2.972854	-4.501739	0.719318
F	-1.043914	4.507454	-2.606851
F	-0.329850	4.672593	1.988918
F	-5.773067	0.145958	2.463251
F	-5.684586	-0.647736	-2.121232

Lowest triplet excited state (T_1)

C	6.002814	-2.133407	0.630129
C	5.448531	-0.948656	0.063777
C	4.065668	-0.798528	-0.057986
C	3.195272	-1.863383	0.361187
C	3.772642	-2.993340	0.969170
C	5.170857	-3.120742	1.088768
H	7.083478	-2.210793	0.700758
C	3.513875	0.416714	-0.575106
C	1.809448	-1.657990	0.128327
H	3.142447	-3.762004	1.405185
H	5.582072	-4.012457	1.555333
C	1.227986	-0.354585	-0.210044
C	2.118981	0.625945	-0.603699
H	1.762769	1.611159	-0.900594
C	4.398901	1.492174	-0.997728
O	3.997169	2.564229	-1.451268
C	6.360951	0.105815	-0.364213
O	7.584307	-0.000906	-0.279786
N	5.773596	1.265231	-0.878332
C	6.639283	2.351255	-1.316324
H	6.447524	2.580841	-2.368046
H	6.438247	3.252473	-0.730179
N	0.843142	-2.666428	0.246917
C	0.939639	-4.054934	0.214610
C	-0.478712	-0.663479	-2.911372
C	-0.552476	1.673757	2.287700
C	-0.461697	-0.543441	3.060819
C	-0.687256	2.504254	1.097170
C	-1.017316	2.542815	-1.305770
C	-4.967507	-0.487891	-1.022633
C	-5.046665	-0.159345	1.315126
H	-3.206955	0.072783	2.360393
C	-3.137087	-0.671975	-3.515028
C	-0.853477	-0.778915	-4.235850
H	0.566922	-0.639599	-2.614227
C	-0.448465	2.127418	3.608445
C	-0.361303	-0.142532	4.377841
H	-0.476296	-1.595393	2.786248
C	-0.649008	3.903182	1.074658
C	-0.971346	3.925720	-1.264414
H	-1.164026	2.060881	-2.272190
C	-5.729141	-0.367514	0.124113
C	-2.211815	-0.778702	-4.538156
H	-4.196797	-0.665875	-3.732442
H	-0.093247	-0.861522	-5.005438
C	-0.355944	1.222930	4.650849
H	-0.449806	3.191340	3.803678
H	-0.289715	-0.886002	5.164610

N	-1.175483	-3.431457	0.346693
C	-0.325796	-4.526414	0.281937
H	1.873042	-4.581968	0.102958
H	-0.698343	-5.540774	0.287430
H	7.671629	2.034310	-1.178631
C	-0.482169	-2.274718	0.302270
Ir	-0.829004	-0.236125	0.073751
C	-2.899574	-0.235788	0.223043
N	-1.370696	-0.551876	-1.909885
N	-0.557412	0.328820	2.040257
C	-0.869498	1.805479	-0.127363
C	-3.569131	-0.421899	-1.015293
C	-3.666130	-0.087307	1.384385
C	-2.709821	-0.558053	-2.186584
C	-0.786110	4.637559	-0.087348
H	-6.811320	-0.424674	0.085973
H	-2.549550	-0.858990	-5.567797
H	-0.282101	1.581600	5.673815
H	-0.748076	5.721068	-0.072864
C	-2.626064	-3.526134	0.399654
H	-3.018778	-2.736112	1.045001
H	-3.056250	-3.412571	-0.600562
H	-2.902830	-4.501702	0.804142
F	-1.110075	4.618232	-2.400604
F	-0.466620	4.601677	2.207453
F	-5.766298	-0.030855	2.435936
F	-5.639522	-0.684952	-2.169111

Complex 5a

Ground-state (S_0)

C	-5.944475	-1.836315	-1.128334
C	-5.381806	-1.028422	-0.161970
C	-3.980388	-0.845063	-0.099446
C	-3.129519	-1.550856	-1.004097
C	-3.754607	-2.318069	-2.019471
C	-5.123452	-2.458055	-2.079250
H	-7.024820	-1.950123	-1.152468
C	-3.424468	0.061436	0.829539
C	-1.726059	-1.362169	-0.840091
H	-3.157681	-2.764362	-2.807442
H	-5.569335	-3.044380	-2.878205
C	-1.164894	-0.379774	-0.019831
C	-2.064498	0.317112	0.814221
H	-1.682239	1.073636	1.500973
C	-4.286099	0.770216	1.783776
O	-3.868753	1.556521	2.621384
C	-6.273634	-0.344042	0.793657
O	-7.485336	-0.508495	0.794027
N	-5.661554	0.508931	1.713650
C	-6.496928	1.211714	2.679697
H	-6.195726	0.949208	3.697277
H	-6.384167	2.291937	2.556650
N	-0.750923	-2.153292	-1.515845
C	-0.826515	-3.379463	-2.169789
N	1.265841	-2.694383	-2.063420
C	0.436759	-3.705979	-2.523366
H	-1.736058	-3.944349	-2.286990
H	0.819626	-4.569530	-3.048322
H	-7.530971	0.919485	2.506268
C	0.559238	-1.743913	-1.411050
Ir	0.922992	-0.088951	-0.218852
C	2.993635	0.035156	-0.378810
N	1.473398	-1.280912	1.387966
N	0.597128	1.321619	-1.697853
C	0.953354	1.624722	0.933639
C	3.650948	-0.694262	0.649892
C	3.833116	0.695754	-1.273216
C	2.824106	-1.376919	1.584969
C	0.652924	-1.891556	2.245672
C	0.562730	2.611631	-1.244004
C	0.459533	1.098328	-3.006886
C	0.738793	2.794175	0.154988
C	1.120000	1.834525	2.300585
C	5.057171	-0.780956	0.782827
C	5.233914	0.617090	-1.171456
H	3.403814	1.286784	-2.086106
C	3.371903	-2.112826	2.657672
C	1.122300	-2.625602	3.336819
H	-0.410771	-1.781544	2.047862
C	0.371891	3.705671	-2.114716
C	0.278107	2.130741	-3.929280
H	0.499310	0.058474	-3.323837
C	0.701381	4.103001	0.689718
C	1.077835	3.125936	2.859290
H	1.290328	0.985647	2.967020
C	5.849099	-0.109402	-0.165430
H	5.850538	1.142750	-1.899889
C	2.483471	-2.739617	3.544503
H	0.407254	-3.096183	4.004091
C	0.229544	3.437873	-3.484603
H	0.174925	1.887305	-4.981953
C	0.873982	4.250038	2.077747
H	1.211449	3.243247	3.934049
H	6.934444	-0.159924	-0.093571
H	2.874002	-3.309316	4.385726
H	0.084056	4.260160	-4.182586
H	0.847079	5.243720	2.522181
C	2.705055	-2.652852	-2.263802
H	2.977312	-1.793160	-2.883779
H	3.219883	-2.564437	-1.302928
H	3.016988	-3.572453	-2.762581
C	0.495300	5.206045	-0.204481
C	0.341107	5.020190	-1.544125
C	4.799673	-2.172276	2.771925
C	5.601545	-1.539974	1.872147
H	5.226906	-2.739304	3.596969
H	6.684907	-1.598511	1.970794
H	0.190872	5.867055	-2.211135
H	0.466743	6.211482	0.214055

Lowest triplet excited state (T_1)

C	-5.969867	-1.617463	-1.319744
C	-5.376931	-0.898566	-0.243131
C	-3.988948	-0.762281	-0.157322
C	-3.152035	-1.391205	-1.143261
C	-3.773429	-2.041333	-2.226240
C	-5.174649	-2.155531	-2.299004
H	-7.052287	-1.701772	-1.345247
C	-3.400953	0.007902	0.896475
C	-1.752235	-1.291321	-0.920726
H	-3.177646	-2.418871	-3.051095
H	-5.620307	-2.672122	-3.145570
C	-1.149670	-0.346633	0.022535
C	-2.010428	0.228907	0.942442
H	-1.630024	0.911632	1.700870
C	-4.252371	0.640665	1.891558
O	-3.822520	1.325267	2.821304
C	-6.254201	-0.299652	0.754697
O	-7.479719	-0.416742	0.719481
N	-5.630640	0.431199	1.770481
C	-6.461274	1.052540	2.792062
H	-6.166656	0.694224	3.782153
H	-6.334877	2.138697	2.773004
N	-0.798780	-2.060893	-1.601371
C	-0.904354	-3.241030	-2.332127
N	1.209633	-2.621107	-2.171122
C	0.354170	-3.579740	-2.692937
H	-1.835300	-3.760609	-2.488431
H	0.717388	-4.419955	-3.267332
H	-7.498028	0.791248	2.587008
C	0.526858	-1.685812	-1.476849
Ir	0.889713	-0.070027	-0.223408
C	2.976889	-0.024010	-0.353531
N	1.393431	-1.343417	1.354790
N	0.645210	1.402207	-1.657827
C	0.979005	1.598727	0.990011
C	3.596921	-0.812163	0.649390
C	3.838536	0.635842	-1.224551
C	2.737979	-1.496617	1.553668
C	0.547063	-1.954052	2.187417
C	0.668089	2.675556	-1.156904
C	0.516878	1.228297	-2.975527
C	0.834738	2.801139	0.249419
C	1.143707	1.747929	2.363007
C	4.997976	-0.955587	0.783914
C	5.235570	0.501418	-1.120942
H	3.434811	1.269526	-2.017522
C	3.253421	-2.291156	2.599935
C	0.983919	-2.746918	3.250144
H	-0.511594	-1.790384	1.999323
C	0.542400	3.806857	-1.991042
C	0.394621	2.299191	-3.861430
H	0.514384	0.199374	-3.328181
C	0.860767	4.090787	0.829157
C	1.164435	3.019929	2.966262
H	1.260747	0.868915	3.000432
C	5.817699	-0.280842	-0.138529
H	5.873996	1.027865	-1.829342
C	2.338474	-2.918804	3.458424
H	0.248167	-3.214812	3.896224
C	0.403413	3.591330	-3.370211
H	0.293022	2.098911	-4.923117
C	1.028183	4.179060	2.222891
H	1.293088	3.092759	4.045278
H	6.899982	-0.373980	-0.065147
H	2.703413	-3.533711	4.278923
H	0.306799	4.443009	-4.040768
H	1.050555	5.156497	2.702009
C	2.650133	-2.607362	-2.372205
H	2.941828	-1.731170	-2.959247
H	3.167089	-2.570195	-1.409261
H	2.937844	-3.514346	-2.906816
C	0.720609	5.232618	-0.028372
C	0.570969	5.101092	-1.374899
C	4.677427	-2.406901	2.718828
C	5.508028	-1.772797	1.847154
H	5.077465	-3.019929	3.524203
H	6.587666	-1.875285	1.948548
H	0.471384	5.977022	-2.012923
H	0.739939	6.223317	0.424050

Complex 3b

Ground-state (S_0)

C	-5.654836	1.588320	0.805121
C	-5.157146	0.507712	0.105742
C	-3.763196	0.341513	-0.065640
C	-2.866853	1.338963	0.419061
C	-3.413027	2.395117	1.189795
C	-4.772107	2.517247	1.377072
H	-6.730349	1.682711	0.928511
C	-3.250582	-0.834245	-0.656540
C	-1.480399	1.128251	0.175139
H	-2.746221	3.105937	1.669618
H	-5.162117	3.332269	1.980890
C	5.366468	-0.096180	-0.629195
C	5.263051	-0.889742	1.636840
H	3.311578	-1.193185	2.469119
C	3.779453	0.706197	-3.083707
C	1.585181	1.100415	-3.960661
H	0.007494	0.707187	-2.532720
C	0.266592	-3.331148	3.010233
C	0.084809	-1.269230	4.213477
H	0.437644	0.475067	2.989373
C	0.774964	-4.588188	0.298636
C	1.334867	-4.191778	-2.003637

C	-0.947406	-0.090699	-0.244653
C	-1.883721	-1.055067	-0.676618
H	-1.531844	-2.015601	-1.055204
C	-4.165230	-1.854716	-1.183829
O	-3.793206	-2.889303	-1.717777
C	-6.102579	-0.487956	-0.433671
O	-7.315208	-0.358387	-0.346475
N	-5.539178	-1.602857	-1.058815
C	-6.426866	-2.619683	-1.609562
H	-6.211768	-2.766056	-2.671154
H	-6.274161	-3.572657	-1.095453
N	-0.495165	2.122785	0.445219
C	-0.514410	3.517236	0.298237
N	1.562032	2.788688	0.731419
C	0.802906	3.935946	0.524044
H	-7.452650	-2.281567	-1.474816
C	0.801791	1.674345	0.614040
Ir	1.135058	-0.324571	0.111484
C	3.176958	-0.467162	0.437890
N	1.861876	0.351932	-1.705226
N	0.623269	-1.255813	1.881485
C	1.152610	-2.287289	-0.489688
C	3.966045	-0.088310	-0.678658
C	3.872100	-0.880133	1.585041
C	3.218303	0.336784	-1.856745
C	1.076499	0.727645	-2.731358
C	0.565756	-2.618677	1.844745
C	0.381501	-0.609440	3.036543
C	0.836535	-3.209260	0.539663
C	1.399785	-2.822646	-1.762142
H	1.650045	-2.156729	-2.590889
C	6.016939	-0.491130	0.530039
H	5.957303	0.209536	-1.492172
H	5.770308	-1.206912	2.547261
C	2.967740	1.084935	-4.137204
H	4.858291	0.683719	-3.205471
H	0.909956	1.390856	-4.758770
C	0.028038	-2.661556	4.196312
H	0.226373	-4.415629	2.976714
H	-0.099069	-0.700476	5.119066
C	1.022833	-5.081367	-0.973094
H	0.527790	-5.282573	1.100803
H	1.528394	-4.574780	-3.004765
H	7.103445	-0.494578	0.573942
H	3.406297	1.366005	-5.090996
H	-0.202351	-3.217181	5.101362
H	0.972603	-6.150528	-1.164918
C	2.993400	2.824613	0.959933
H	3.328061	1.831109	1.261729
H	3.522608	3.120566	0.046464
H	3.217398	3.544150	1.753489
C	1.181611	5.269906	0.457079
C	0.197554	6.190586	0.114047
C	-1.485366	4.438954	-0.087375
C	-1.107643	5.775637	-0.169156
H	2.208032	5.577796	0.638687
H	-2.496831	4.136788	-0.336644
H	-1.848196	6.512064	-0.470015
H	0.452406	7.244690	0.044533

Lowest triplet excited state (T_1)

C	-5.654461	1.331835	0.956784
C	-5.108828	0.272064	0.177028
C	-3.731702	0.183514	-0.034039
C	-2.869460	1.205806	0.492045
C	-3.430282	2.200787	1.313635
C	-4.819697	2.259786	1.529678
H	-6.731221	1.362532	1.096527
C	-3.173359	-0.927273	-0.746805
C	-1.501176	1.096945	0.134728
H	-2.781313	2.920555	1.805073
H	-5.225912	3.046617	2.160642
C	-0.905509	-0.159964	-0.306013
C	-1.777760	-1.106688	-0.817809
H	-1.404754	-2.049752	-1.215626
C	-4.052462	-1.947537	-1.293545
O	-3.651516	-2.934346	-1.912530
C	-6.017077	-0.723314	-0.379299
O	-7.238245	-0.667038	-0.231563
N	-5.427712	-1.765262	-1.102715
C	-6.290272	-2.784958	-1.682248
H	-6.084484	-2.881483	-2.751374
H	-6.101628	-3.754959	-1.212338
N	-0.560461	2.131577	0.280982
C	-0.670019	3.523842	0.148345
N	1.476827	2.909355	0.389284
C	0.638006	4.012414	0.245338
H	-7.324101	-2.485915	-1.517844
C	0.772097	1.757699	0.367878
Ir	1.129835	-0.283935	0.098618
C	5.316466	-0.067240	-0.913057
C	5.348455	-0.504173	1.450429
H	3.451301	-0.728353	2.421385
C	3.584722	0.296119	-3.369510
C	1.341339	0.472017	-4.184440
H	-0.155674	0.255483	-2.642299
C	0.579103	-2.776484	3.511447
C	0.454653	-0.544726	4.373340
H	0.660160	0.977637	2.857478
C	0.887841	-4.460604	1.008689
C	1.306008	-4.444467	-1.357688
H	1.542607	-2.529371	-2.289640
C	6.033654	-0.261598	0.257738
H	5.853435	0.117175	-1.842676
H	5.908401	-0.664566	2.370716
C	2.713202	0.476085	-4.427537
H	4.657336	0.289522	-3.537851
H	0.617843	0.607424	-4.981516
C	0.430455	-1.922060	4.588026
H	0.568419	-3.851977	3.659734
H	0.342092	0.163648	5.187253
C	1.068991	-5.153521	-0.178289
H	0.698451	-5.015111	1.926877
H	1.449462	-4.985307	-2.291940
H	7.120330	-0.229705	0.244373
H	3.097166	0.615856	-5.434405
H	0.298648	-2.323317	5.589165
H	1.025081	-6.239786	-0.189281
C	2.917899	3.024885	0.507965

C	3.200125	-0.325213	0.311005
N	1.746555	0.104149	-1.854249
N	0.776332	-0.912775	2.031766
C	1.171084	-2.321410	-0.170421
C	3.915986	-0.103643	-0.888949
C	3.957020	-0.539561	1.471856
C	3.093439	0.108030	-2.074015
C	0.902968	0.283327	-2.888381
C	0.754409	-2.264386	2.222218
C	0.628314	-0.085080	3.083514
C	0.938704	-3.060414	1.015278
C	1.357887	-3.053366	-1.349699
H	3.329617	2.047210	0.763548
H	3.354058	3.368885	-0.436737
H	3.162277	3.742503	1.297052
C	0.934221	5.365053	0.146764
C	-0.131382	6.228086	-0.083463
C	-1.729288	4.386984	-0.119515
C	-1.435934	5.742431	-0.226841
H	1.954500	5.731118	0.225074
H	-2.743476	4.023346	-0.247204
H	-2.243736	6.439617	-0.432707
H	0.054880	7.295086	-0.170780

Complex 4b

Ground-state (S_0)

C	-6.002615	1.449914	0.787806
C	-5.437024	0.374932	0.133714
C	-4.035091	0.291864	-0.034669
C	-3.204014	1.364370	0.405271
C	-3.816912	2.414300	1.133103
C	-5.180992	2.456719	1.317725
H	-7.081728	1.480157	0.911545
C	-3.449770	-0.873043	-0.576483
C	-1.806441	1.231485	0.167010
H	-3.198009	3.184556	1.584151
H	-5.622842	3.269560	1.887761
C	-1.200783	0.032319	-0.207419
C	-2.072461	-1.007805	-0.594316
H	-1.662707	-1.959525	-0.935918
C	-4.296896	-1.974028	-1.053154
O	-3.857680	-3.003994	-1.543051
C	-6.316506	-0.703302	-0.356614
O	-7.534672	-0.647743	-0.271363
N	-5.683104	-1.807815	-0.930929
C	-6.504136	-2.904823	-1.429178
H	-6.283892	-3.084547	-2.484470
H	-6.286143	-3.820490	-0.872784
N	-0.880319	2.292217	0.393600
C	-0.979830	3.679441	0.214914
N	1.136470	3.081100	0.658411
C	0.311847	4.177874	0.426494
H	-7.549567	-2.629463	-1.302740
C	0.439523	1.925387	0.569115
Ir	0.891242	-0.062946	0.125698
C	2.938729	-0.073297	0.427979
N	1.554573	0.596050	-1.721326
N	0.464898	-0.969237	1.929123
C	1.014084	-2.033210	-0.420950
C	3.688263	0.312263	-0.719490
C	3.636229	-0.415015	1.592925
C	2.907879	0.645942	-1.906732
C	0.723896	0.882295	-2.740209
C	0.489005	-2.335593	1.943235
C	0.223555	-0.291779	3.065971
C	0.762781	-2.940698	0.645177
C	1.269721	-2.551720	-1.694931
C	5.083269	0.367800	-0.628686
C	5.018631	-0.347350	1.620664
H	3.116599	-0.729302	2.498490
C	3.414996	0.978357	-3.169600
C	1.177980	1.218407	-4.000843
H	-0.336751	0.817697	-2.510252
C	0.272622	-3.015884	3.147765
C	0.005455	-0.918377	4.277534
H	0.219432	0.791422	2.976494
C	0.774058	-4.314297	0.378960
C	1.267306	-3.921133	-1.896034
H	1.471130	-1.905515	-2.549478
C	5.773964	0.049706	0.525288
C	2.552747	1.259287	-4.214738
H	4.485882	1.002051	-3.321486
H	0.466640	1.434126	-4.791101
C	0.033859	-2.309526	4.313272
H	0.298993	-4.097201	3.155614
H	-0.181376	-0.324942	5.166361
C	1.021569	-4.832111	-0.877844
H	6.856383	0.103375	0.563614
H	2.952757	1.508764	-5.193854
H	-0.129691	-2.841823	5.246408
H	1.019983	-5.902109	-1.053786
C	2.562791	3.201446	0.890504
H	2.944998	2.242575	1.244707
H	3.083464	3.481406	-0.032713
H	2.743431	3.967075	1.651097
F	1.511358	-4.401678	-3.121211
F	0.531072	-5.203278	1.357520
F	5.667905	-0.668055	2.746630
F	5.824357	0.750206	-1.683031
C	-2.002690	4.535639	-0.186918
C	0.615062	5.529187	0.328429
C	-0.420779	6.384335	-0.029157
C	-1.701367	5.889347	-0.298017
H	-2.995780	4.170748	-0.426446
H	1.623340	5.897946	0.497735
H	-0.226994	7.449414	-0.123545
H	-2.483270	6.576062	-0.611388

Lowest triplet excited state (T_1)

C	-5.978210	1.259757	0.940811
C	-5.380854	0.214236	0.178245
C	-4.002106	0.189486	-0.031839
C	-3.189679	1.260347	0.475662
C	-3.797555	2.239868	1.280770
C	-5.189591	2.235159	1.497125
H	-7.054913	1.239935	1.081418
C	-3.390517	-0.907597	-0.721147
C	-1.815616	1.206113	0.126606
H	-3.185054	2.997386	1.761855
H	-5.632890	3.012459	2.114566
C	-1.159128	-0.030313	-0.297820
C	-1.985774	-1.025296	-0.785085
H	-1.571841	-1.958888	-1.164557
C	-4.219589	-1.979590	-1.249279
O	-3.768669	-2.955729	-1.849405
C	-6.239987	-0.835816	-0.358259
O	-7.461651	-0.834072	-0.210383
N	-5.601004	-1.862581	-1.060029
C	-6.411882	-2.936785	-1.615967
H	-6.232164	-3.021379	-2.690992
H	-6.144861	-3.890341	-1.151346
N	-0.921358	2.280343	0.261521
C	-1.086512	3.668078	0.129204
N	1.081665	3.141895	0.395159
C	0.199214	4.209388	0.240378
H	-7.457504	-2.704163	-1.421994
C	0.425669	1.963963	0.359726
Ir	0.885246	-0.052250	0.087355
C	2.948254	0.007552	0.325147
N	1.497823	0.384159	-1.852394
N	0.536373	-0.710405	2.010387
C	1.021692	-2.078796	-0.196485
C	3.660334	0.279653	-0.873912
C	3.672649	-0.183799	1.506819
C	2.845272	0.456472	-2.070807
C	0.643028	0.523870	-2.882869
C	0.559583	-2.063874	2.201181
C	0.348381	0.114440	3.056788
C	0.797974	-2.835253	0.986863
C	1.266359	-2.758465	-1.392356
C	5.055035	0.381838	-0.820951
C	5.052947	-0.074134	1.496754
H	3.179545	-0.408633	2.452694
C	3.321029	0.668049	-3.370715
C	1.066073	0.735854	-4.180411
H	-0.412096	0.443709	-2.633333
C	0.381117	-2.576907	3.491925
C	0.172749	-0.345161	4.346298
H	0.350927	1.176493	2.825894
C	0.823327	-4.232001	0.906488
C	1.278450	-4.143214	-1.408656
H	1.446834	-2.229128	-2.327494
C	5.774601	0.216845	0.347301
C	2.434306	0.804777	-4.423871
H	4.387850	0.714083	-3.543119
H	0.334520	0.838118	-4.974981
C	0.189800	-1.720685	4.561578
H	0.401238	-3.647871	3.643164
H	0.027923	0.361903	5.156141
C	1.058573	-4.910695	-0.273433
H	6.855485	0.303025	0.355595
H	2.810424	0.962187	-5.431075
H	0.056951	-2.125555	5.561111
H	1.068131	-5.994519	-0.303684
C	2.517431	3.310160	0.522030
H	2.948551	2.387562	0.915166
H	2.968596	3.535370	-0.450881
H	2.725449	4.129454	1.215842
F	1.511304	-4.780280	-2.561320
F	0.610869	-4.983462	1.999306
F	5.731472	-0.245479	2.636815
F	5.765751	0.660512	-1.926075
C	-2.176021	4.488301	-0.152854
C	0.443393	5.572089	0.140382
C	-0.652586	6.391533	-0.104063
C	-1.935139	5.854035	-0.260678
H	-3.173411	4.085081	-0.292957
H	1.448277	5.976797	0.226623
H	-0.507777	7.464689	-0.193464
H	-2.767601	6.517485	-0.479036

Complex 5b

Ground-state (S_0)

C	5.806913	1.852779	-0.635692
C	5.298263	0.831038	0.139778
C	3.901986	0.630642	0.239471
C	3.008382	1.536450	-0.405122
C	3.571406	2.528390	-1.245887
C	4.935552	2.684207	-1.356179
H	6.884841	1.973991	-0.700685
C	3.388499	-0.493249	0.922299
C	1.616189	1.298557	-0.229383
H	2.916441	3.158088	-1.841449
H	5.339519	3.447064	-2.016324
H	-3.084213	-1.462519	-2.499915
C	-3.856440	1.058039	2.707685
C	-1.745309	1.621251	3.715210
H	-0.016153	1.117161	2.494460
C	0.198583	-3.553418	-2.608391
C	0.343051	-1.660874	-4.086226
H	-0.158897	0.236907	-3.155543
C	-0.391337	-4.489395	0.020924
C	-1.094807	-3.963424	2.264660
H	-1.549144	-1.906138	2.710943
C	-5.832517	-0.627107	-0.665708

C	1.096193	0.111771	0.288078
C	2.031105	-0.763448	0.881610
H	1.686681	-1.691434	1.339574
C	4.296941	-1.417612	1.611720
O	3.920677	-2.400330	2.233454
C	6.236526	-0.068178	0.837605
O	7.447751	0.097056	0.812020
N	5.668191	-1.133308	1.540484
C	6.548732	-2.056103	2.246727
H	6.286625	-2.084701	3.307526
H	6.439555	-3.064773	1.839179
N	0.617891	2.217569	-0.668000
C	0.577778	3.619502	-0.687048
N	-1.440257	2.755819	-1.153518
C	-0.737248	3.950866	-1.037456
H	7.572683	-1.708993	2.121261
C	-0.648359	1.698043	-0.861711
Ir	-0.947129	-0.240874	-0.159006
C	-2.970514	-0.502189	-0.572541
N	-1.769546	0.594775	1.554280
N	-0.325480	-1.316746	-1.814318
C	-0.932055	-2.131884	0.656636
C	-3.794692	-0.020980	0.481829
C	-3.647401	-1.060866	-1.654507
C	-3.135661	0.553756	1.603746
C	-1.100090	1.115155	2.584605
C	-0.208028	-2.661209	-1.594201
C	-0.052841	-0.837965	-3.029503
C	-0.517232	-3.114451	-0.282079
C	-1.218711	-2.600305	1.935528
C	-5.207931	-0.067640	0.463887
C	-5.053332	-1.116678	-1.699747
C	-3.125337	1.595395	3.778037
H	-1.150013	2.029109	4.525814
C	0.471793	-3.020815	-3.877511
H	0.546476	-1.215853	-5.055051
C	-0.688905	-4.902335	1.332262
H	-6.919285	-0.675188	-0.712297
H	-3.651694	1.987089	4.646459
H	0.783795	-3.682175	-4.683623
H	-0.599745	-5.954096	1.599452
C	-2.855426	2.699222	-1.464015
H	-3.125842	1.665999	-1.689163
H	-3.451428	3.050922	-0.613394
H	-3.063851	3.328365	-2.334646
C	1.486364	4.624422	-0.360002
C	-1.171292	5.264433	-1.152741
C	-0.246952	6.262866	-0.868000
C	1.052727	5.942979	-0.462467
H	2.491934	4.401555	-0.018800
H	-2.196094	5.500189	-1.427886
H	-0.545315	7.305370	-0.938845
H	1.745135	6.742372	-0.211802
H	-1.325922	-4.286633	3.278898
H	-5.539961	-1.555612	-2.570097
C	-5.929530	0.454318	1.589085
C	-5.287301	0.988698	2.663680
C	0.029546	-5.385747	-1.017382
C	0.307776	-4.943102	-2.274428
H	-7.017881	0.412216	1.569228
H	-5.848040	1.376642	3.512089
H	0.623386	-5.636320	-3.051937
H	0.121951	-6.444691	-0.779041

Lowest triplet excited state (T_1)

C	5.881317	1.436525	-0.712256
C	5.283253	0.479938	0.157844
C	3.894734	0.395720	0.271486
C	3.069031	1.317100	-0.459349
C	3.686349	2.198848	-1.366191
C	5.088336	2.258838	-1.473860
H	6.965338	1.471186	-0.766463
C	3.290298	-0.616533	1.086322
C	1.676918	1.231115	-0.203178
H	3.073023	2.828549	-2.005009
H	5.537503	2.961148	-2.171845
C	1.055017	0.044703	0.380761
C	1.893855	-0.803993	1.083327
H	1.499607	-1.684940	1.587237
C	4.131239	-1.543396	1.826026
O	3.689866	-2.444204	2.541157
C	6.152108	-0.418351	0.908457
O	7.380716	-0.358079	0.850289
N	5.515699	-1.372644	1.708666
C	6.337051	-2.299233	2.474356
H	6.130000	-2.191040	3.542992
H	6.106837	-3.328925	2.187539
N	0.741425	2.204041	-0.595405
C	0.821417	3.602091	-0.686090
N	-1.283113	2.897499	-1.029471
C	-0.475297	4.032173	-0.989748
H	7.381628	-2.072634	2.267594
H	-3.199814	-1.106700	-2.502642
C	-3.716712	0.994274	2.916556
C	-1.558094	1.351845	3.914966
H	0.116231	0.867382	2.618711
C	-0.080473	-3.313219	-2.923575
C	0.142340	-1.304034	-4.229277
H	-0.210396	0.526772	-3.119399
C	-0.664366	-4.453402	-0.376057
C	-1.270262	-4.098365	1.928667
H	-1.555949	-2.066400	2.582826
C	-5.856388	-0.306315	-0.524470
C	-2.935452	1.392934	4.011365
H	-0.924031	1.647317	4.744577
C	0.189522	-2.683009	-4.147341
H	0.345301	-0.785883	-5.160945
C	-0.959860	-4.968474	0.898897
H	-6.944960	-0.304621	-0.540631
H	-3.420949	1.727391	4.926176
H	0.434064	-3.284772	-5.020543
H	-0.941231	-6.044670	1.062284
C	-2.709888	2.952908	-1.283714
H	-3.079720	1.937396	-1.434575
H	-3.232344	3.409384	-0.435330
H	-2.898282	3.546891	-2.183052
C	1.837394	4.526146	-0.456922
C	-0.794133	5.374329	-1.144233
C	0.233118	6.292215	-0.954796

C	-0.572529	1.785554	-0.744483
Ir	-0.937624	-0.179101	-0.145015
C	-2.996310	-0.309620	-0.508212
N	-1.682512	0.537627	1.668467
N	-0.429269	-1.131244	-1.913299
C	-1.016077	-2.139434	0.495732
C	-3.763892	0.118437	0.605451
C	-3.721437	-0.750158	-1.611826
C	-3.047549	0.561171	1.751776
C	-0.964891	0.920207	2.727153
C	-0.394433	-2.495960	-1.817488
C	-0.168310	-0.559349	-3.090824
C	-0.695319	-3.049840	-0.543670
C	-1.301724	-2.704224	1.733776
C	-5.177637	0.131464	0.627359
C	-5.129629	-0.742121	-1.618251
C	1.520975	5.872396	-0.603646
H	2.836030	4.216904	-0.167877
H	-1.805457	5.694362	-1.380521
H	0.027142	7.353698	-1.062904
H	2.295631	6.615549	-0.434429
H	-1.496801	-4.500962	2.914906
H	-5.658534	-1.086465	-2.506007
C	-5.845194	0.585116	1.813387
C	-5.149901	0.994748	2.909325
C	-0.335603	-5.273377	-1.506450
C	-0.058902	-4.732596	-2.724501
H	-6.934260	0.591894	1.823283
H	-5.668470	1.330521	3.805344
H	0.187439	-5.367125	-3.573634
H	-0.311870	-6.353878	-1.371270

NMR Spectra

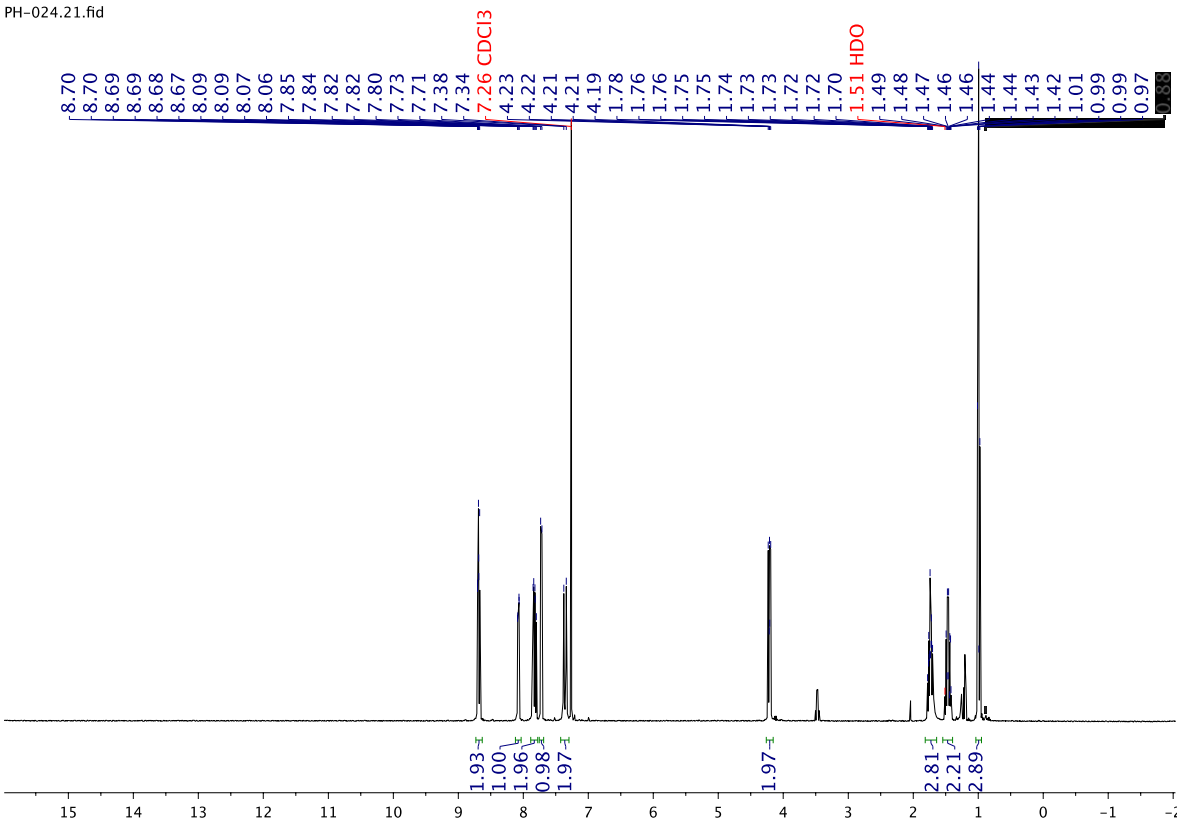


Figure S10. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1a**

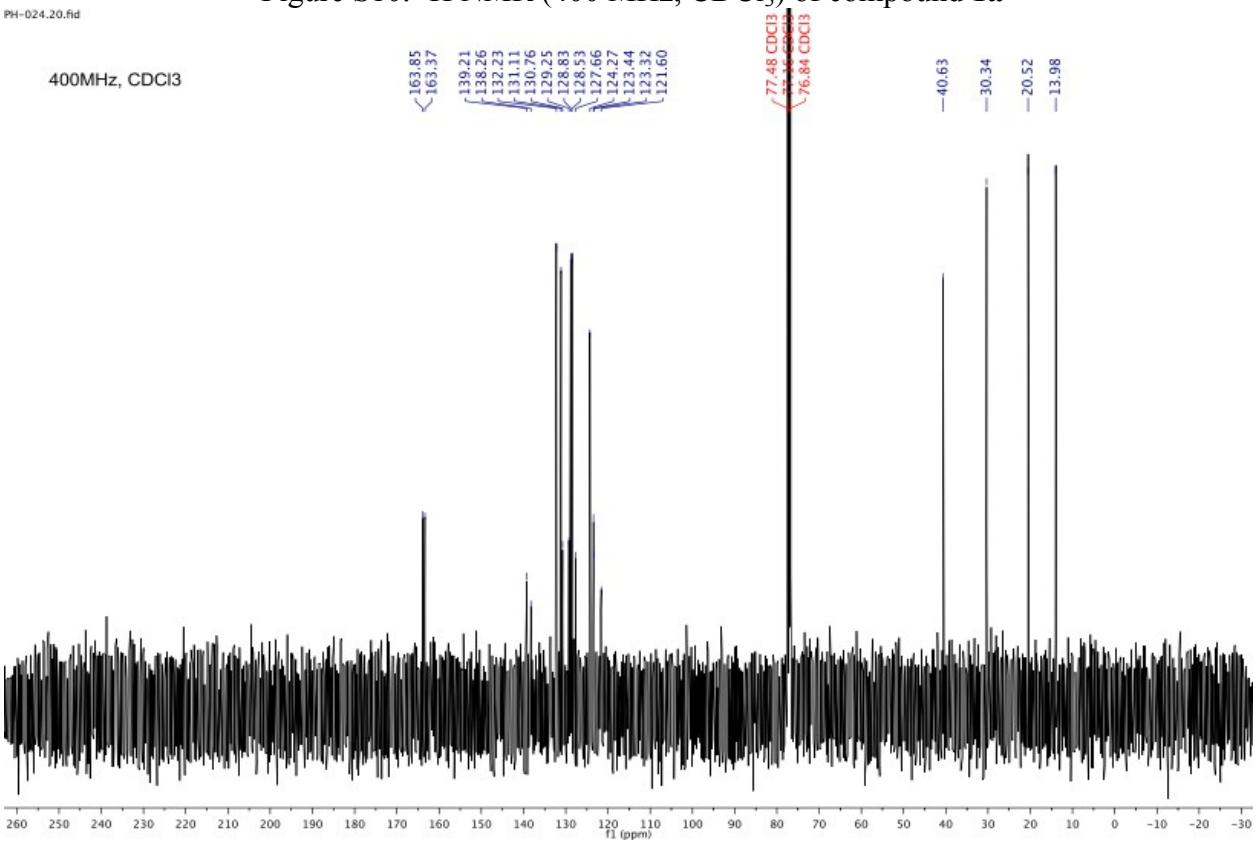


Figure S11. ^{13}C NMR (101 MHz, $CDCl_3$) of compound **1a**

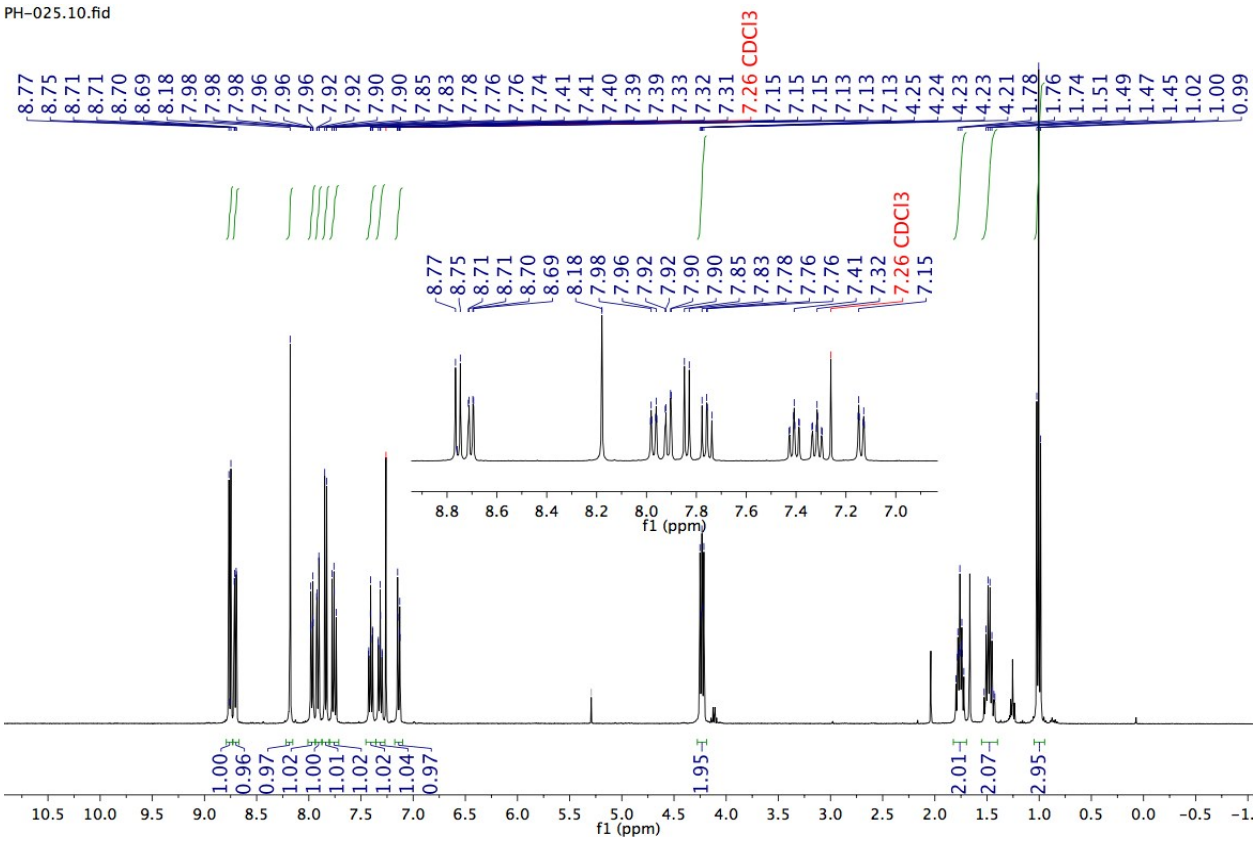


Figure S12. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **1b**

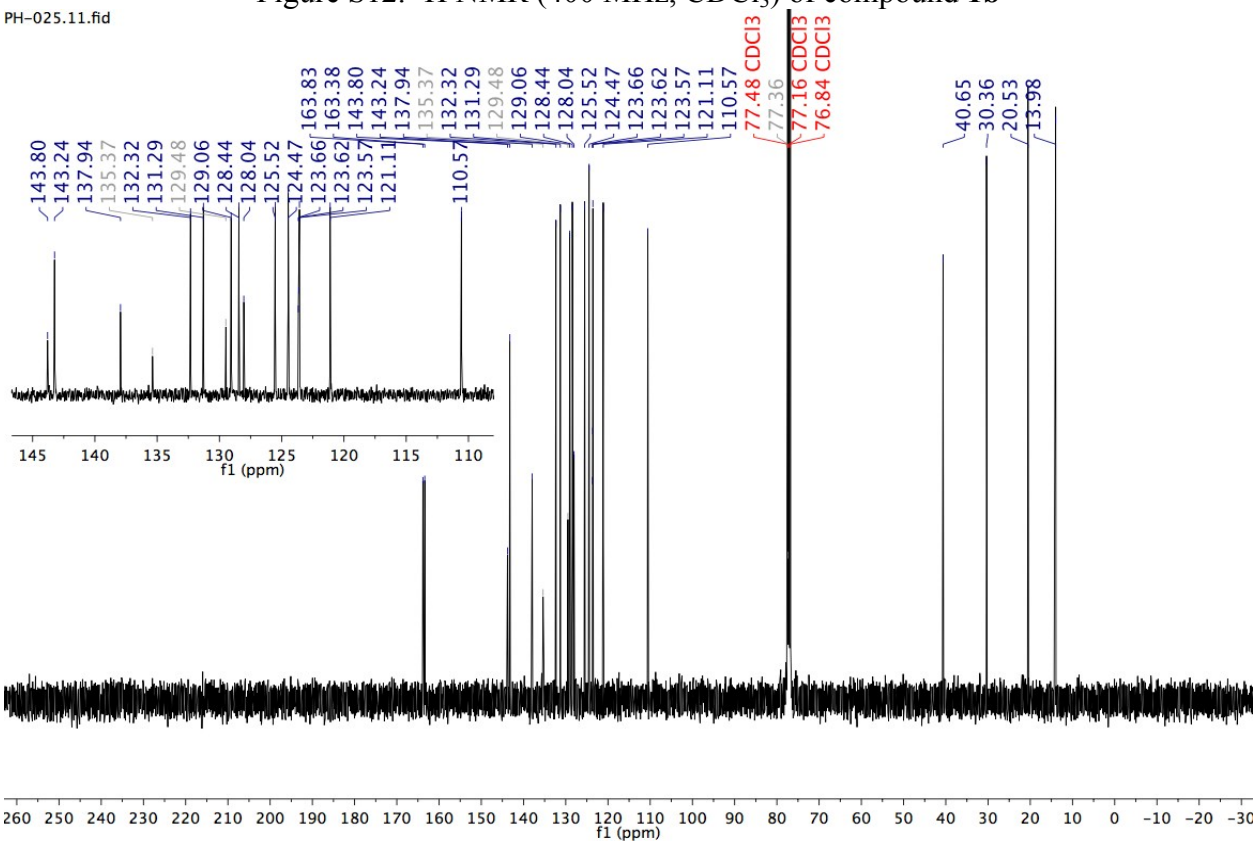


Figure S13. ^{13}C NMR (101 MHz, $CDCl_3$) of compound **1b**

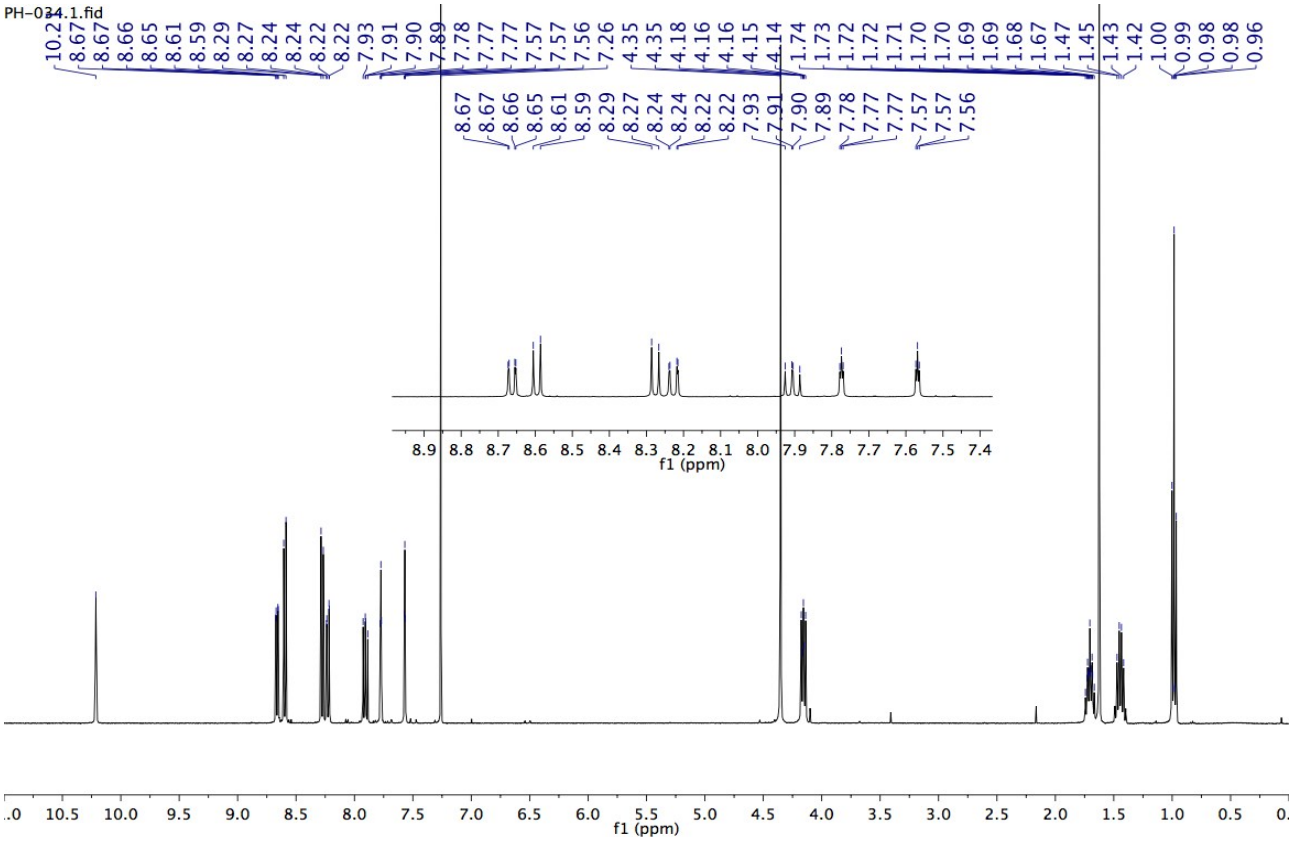


Figure S14. ^{1}H NMR (400 MHz) of compound **2a**

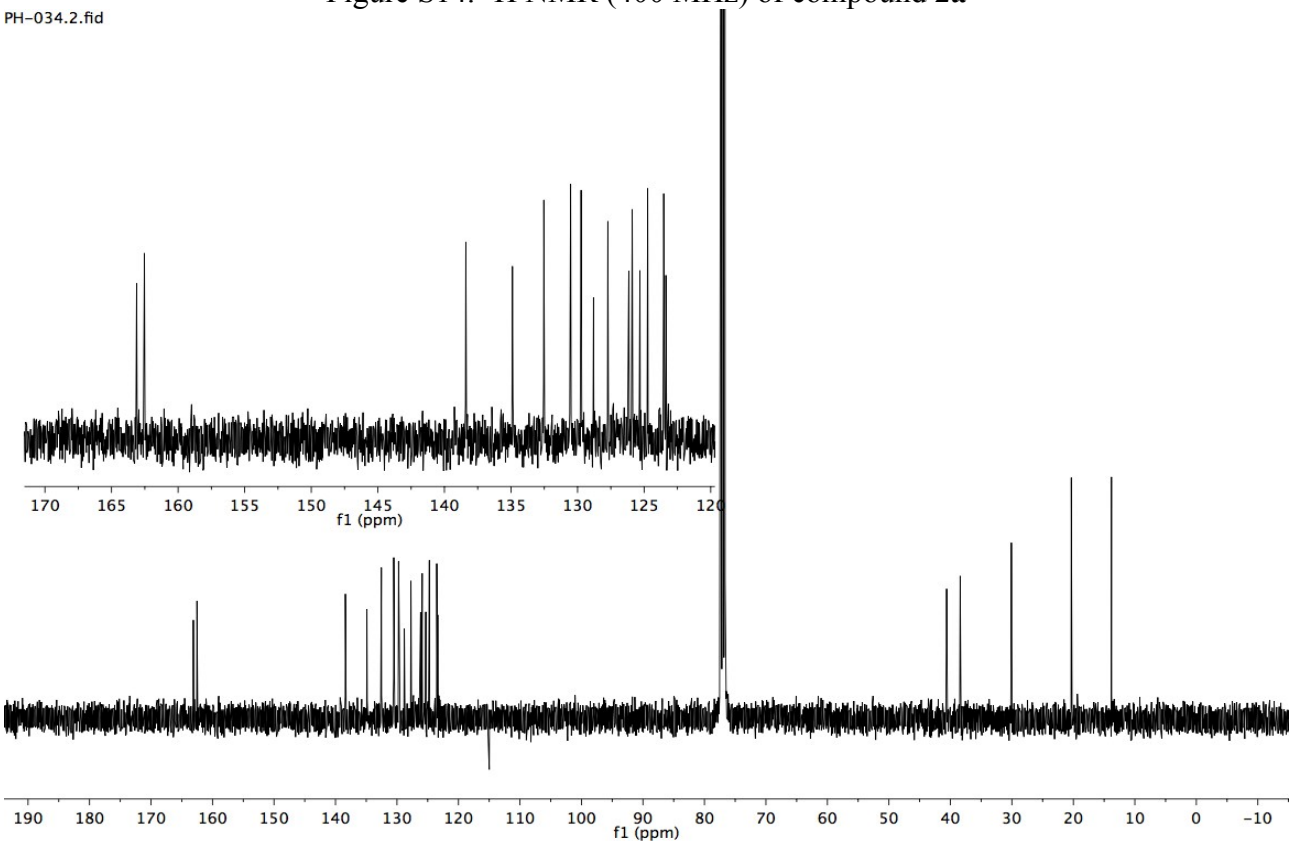


Figure S15. ^{13}C NMR (100 MHz, $CDCl_3$) of compound **2a**

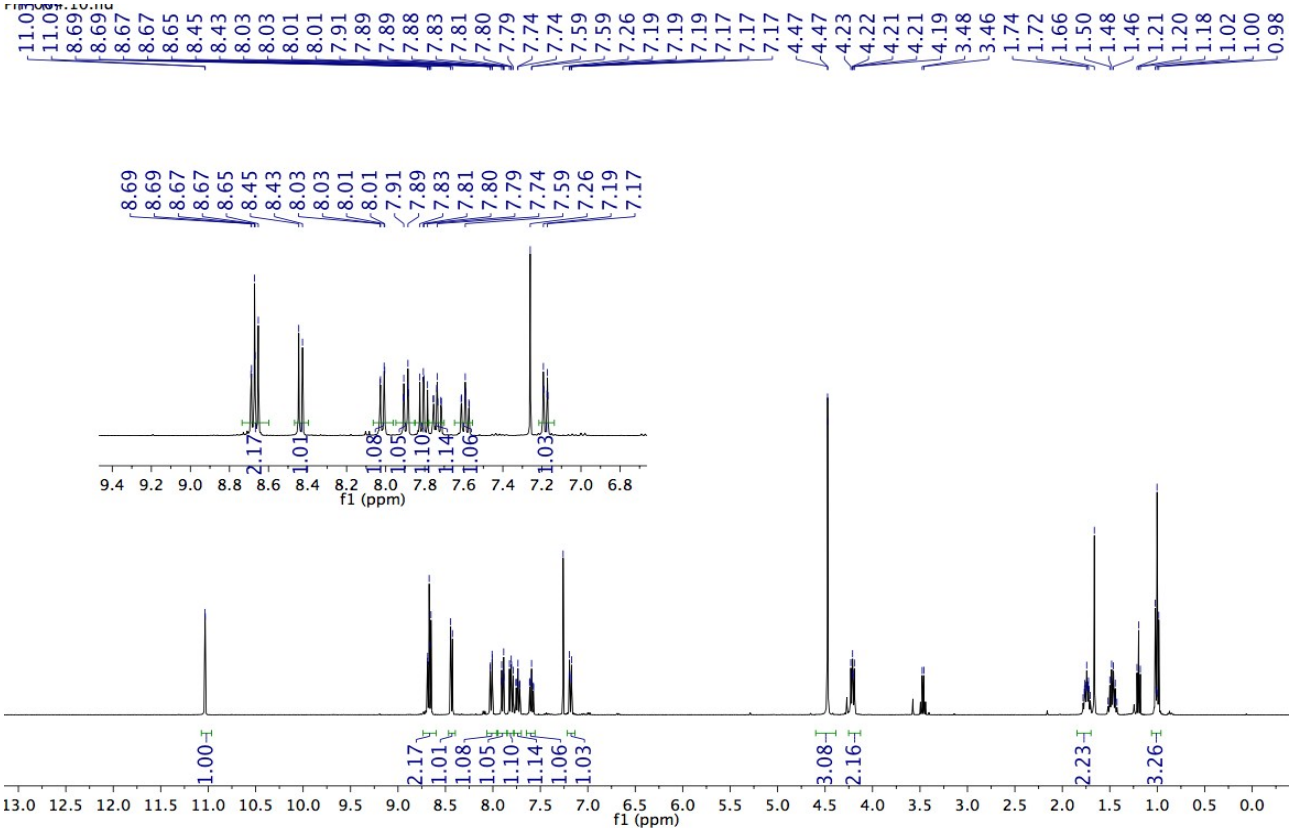


Figure S16. ^{1}H NMR (400 MHz, $CDCl_3$) of compound **2b**

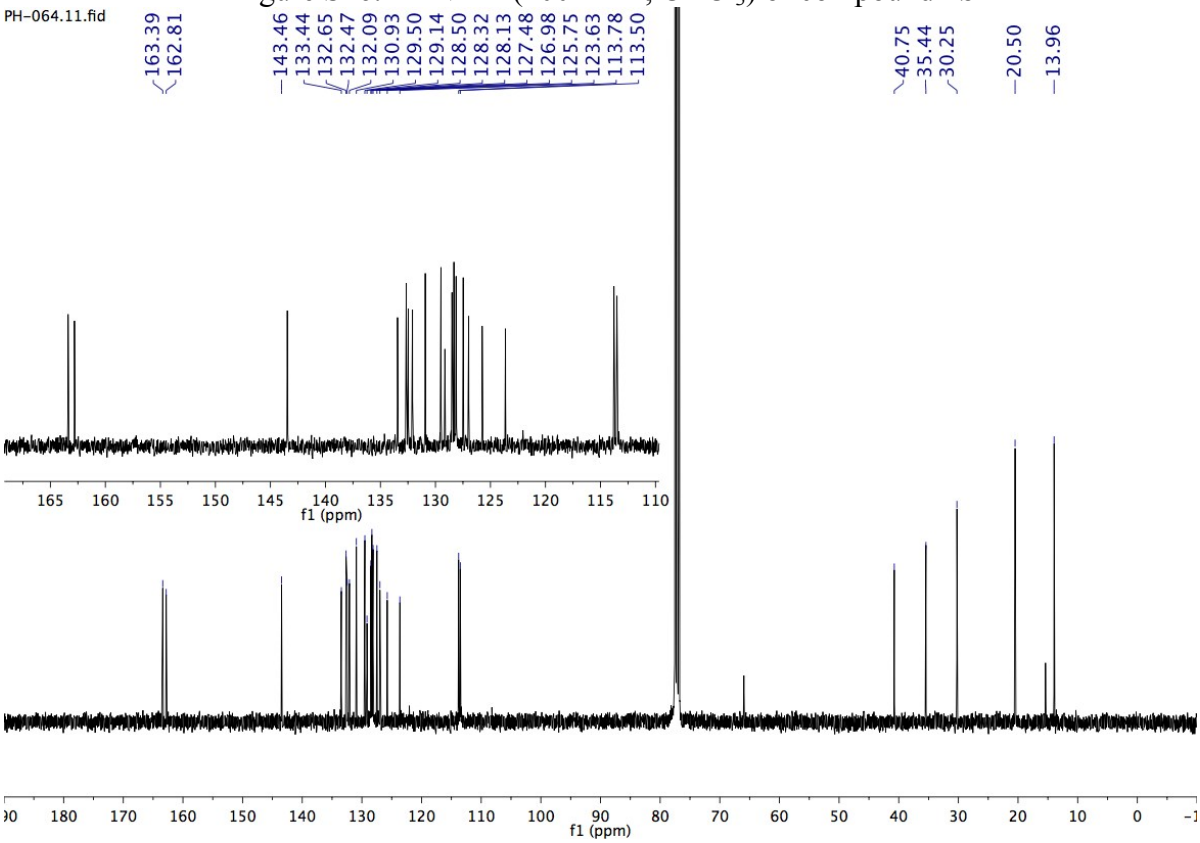


Figure S17. ^{13}C NMR (100 MHz, $CDCl_3$) of compound **2b**

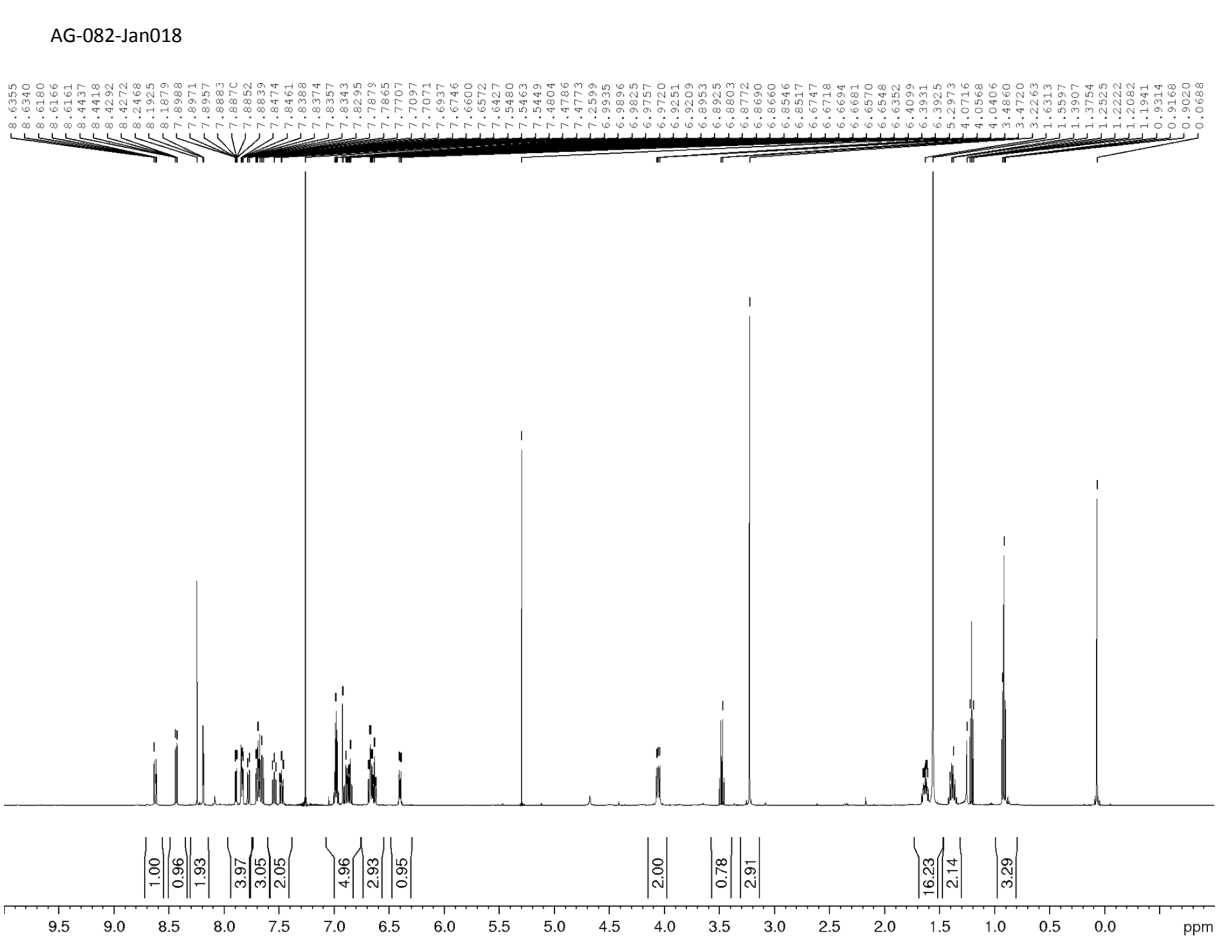


Figure S18. ^{1}H NMR (500 MHz, $CDCl_3$) of compound **3a**

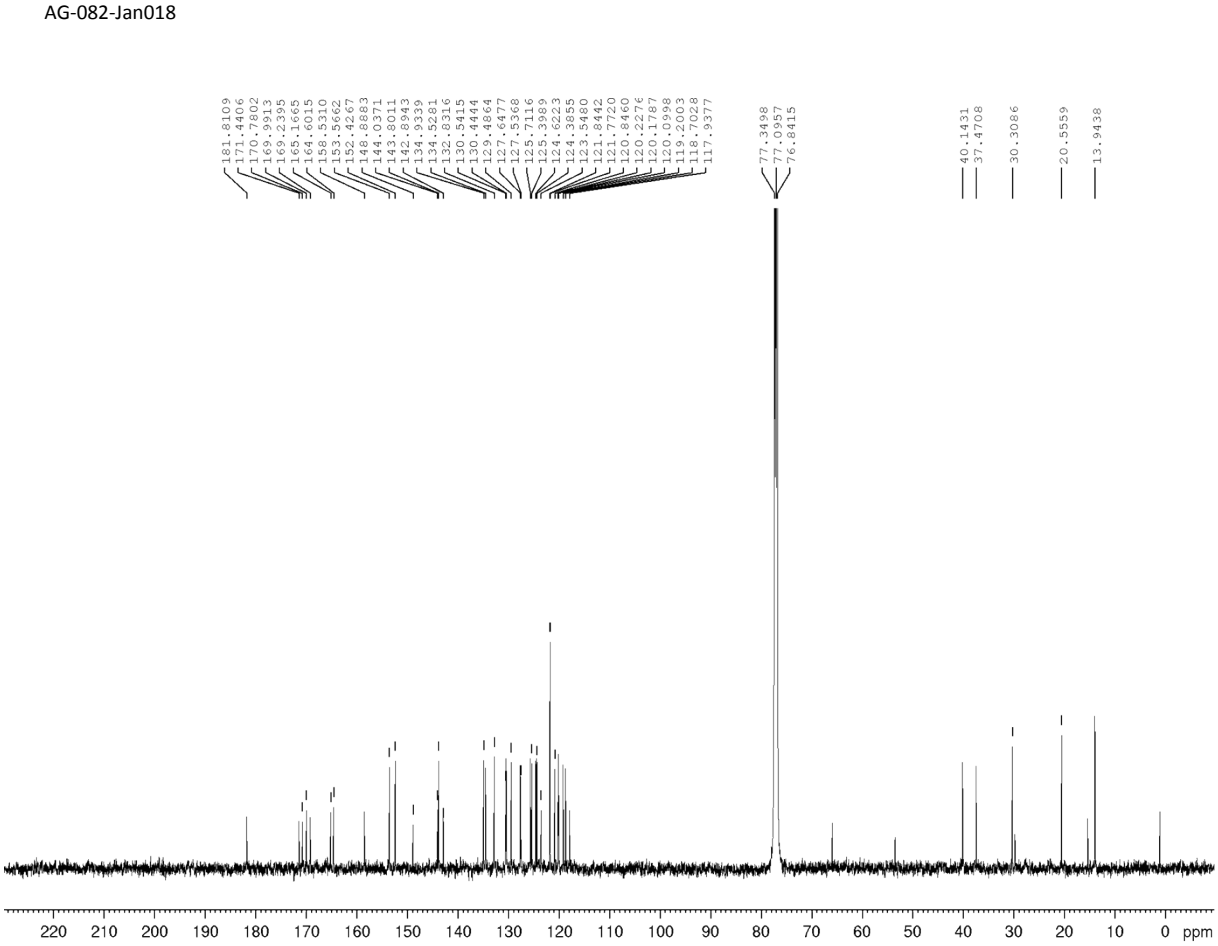


Figure S19.^{13}C NMR (125 MHz, $CDCl_3$) of compound **3a**

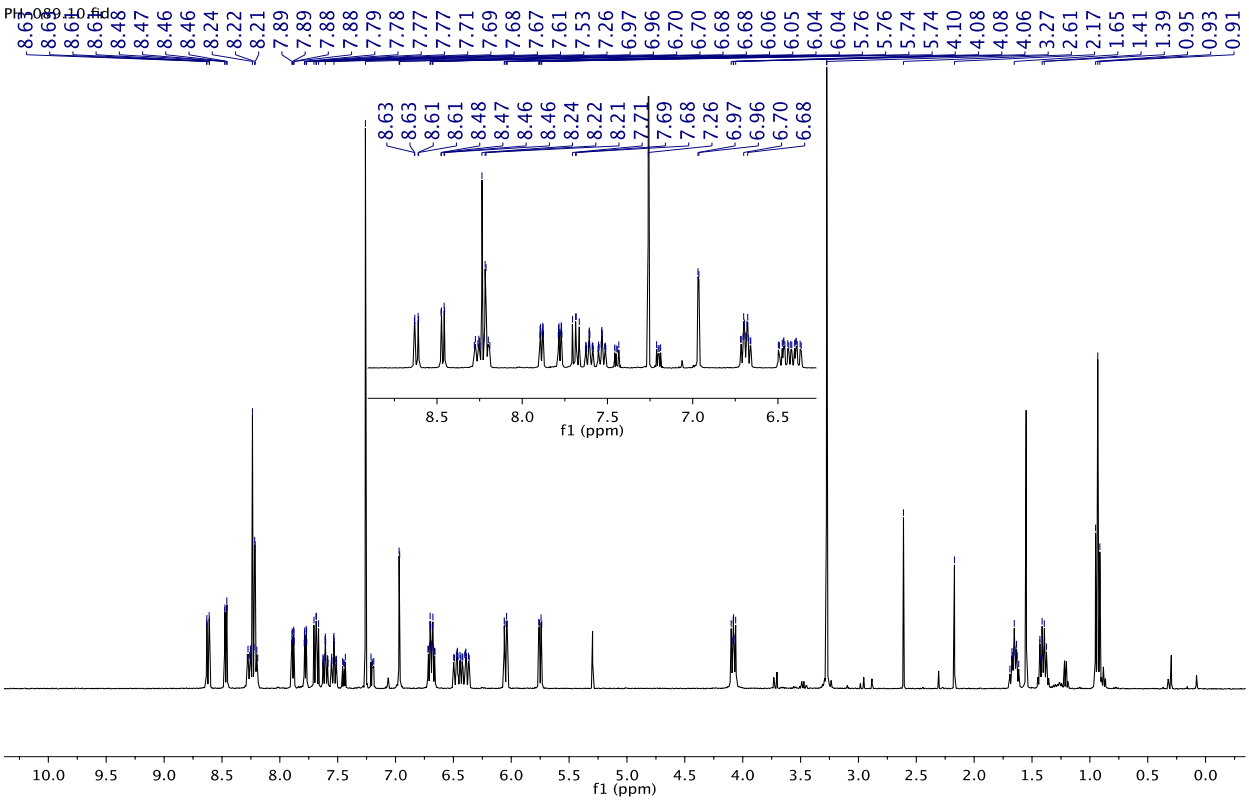


Figure S20. ^{1}H NMR (400 MHz) Compound **4a**

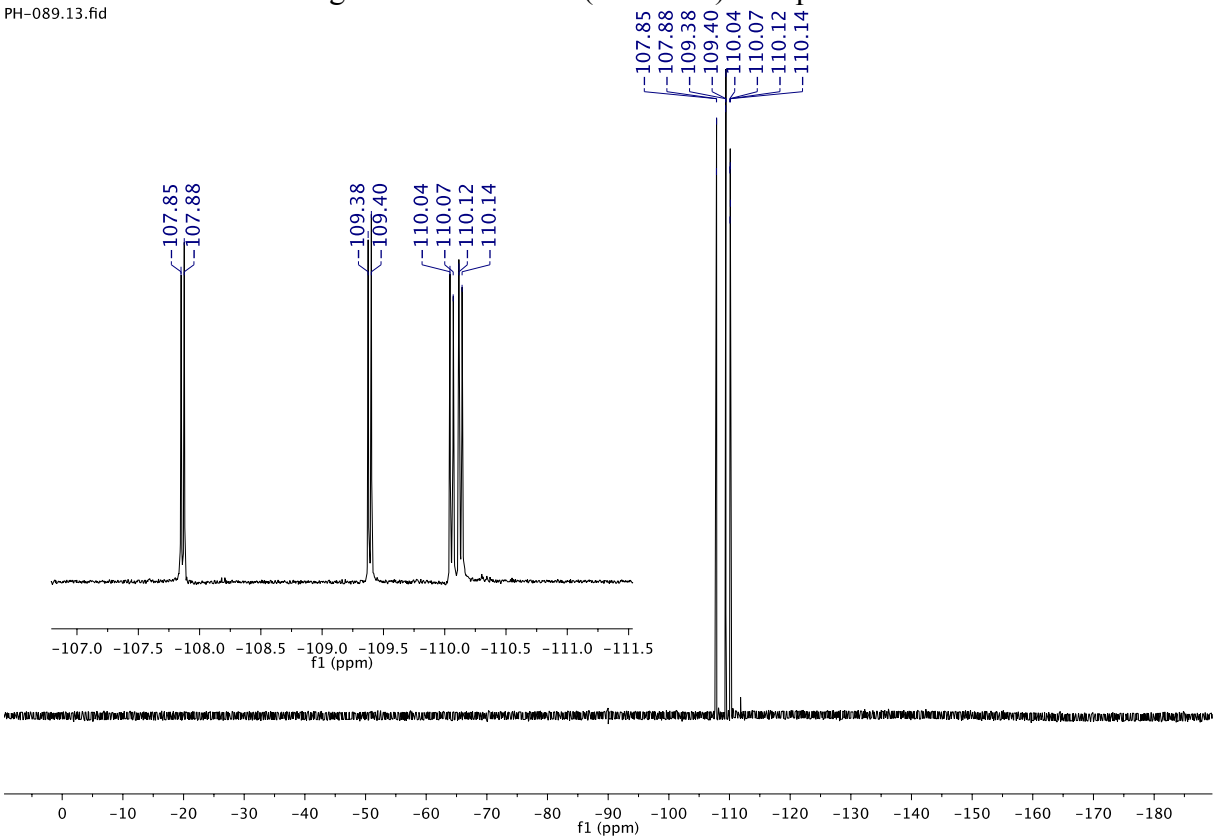


Figure S21. ^{19}F NMR (376 MHz) Compound **4a**

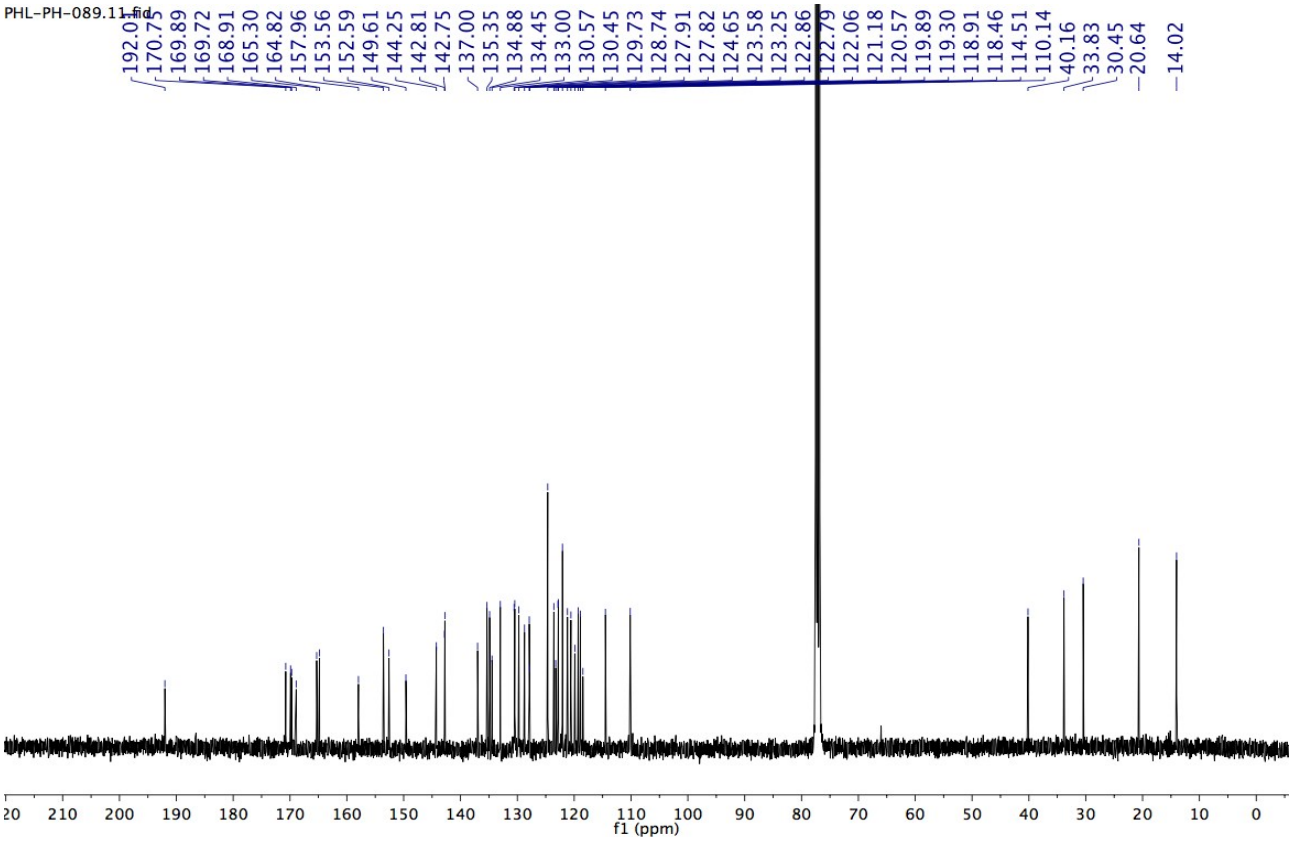


Figure S22.[13]C NMR (101 MHz) Compound **4a**

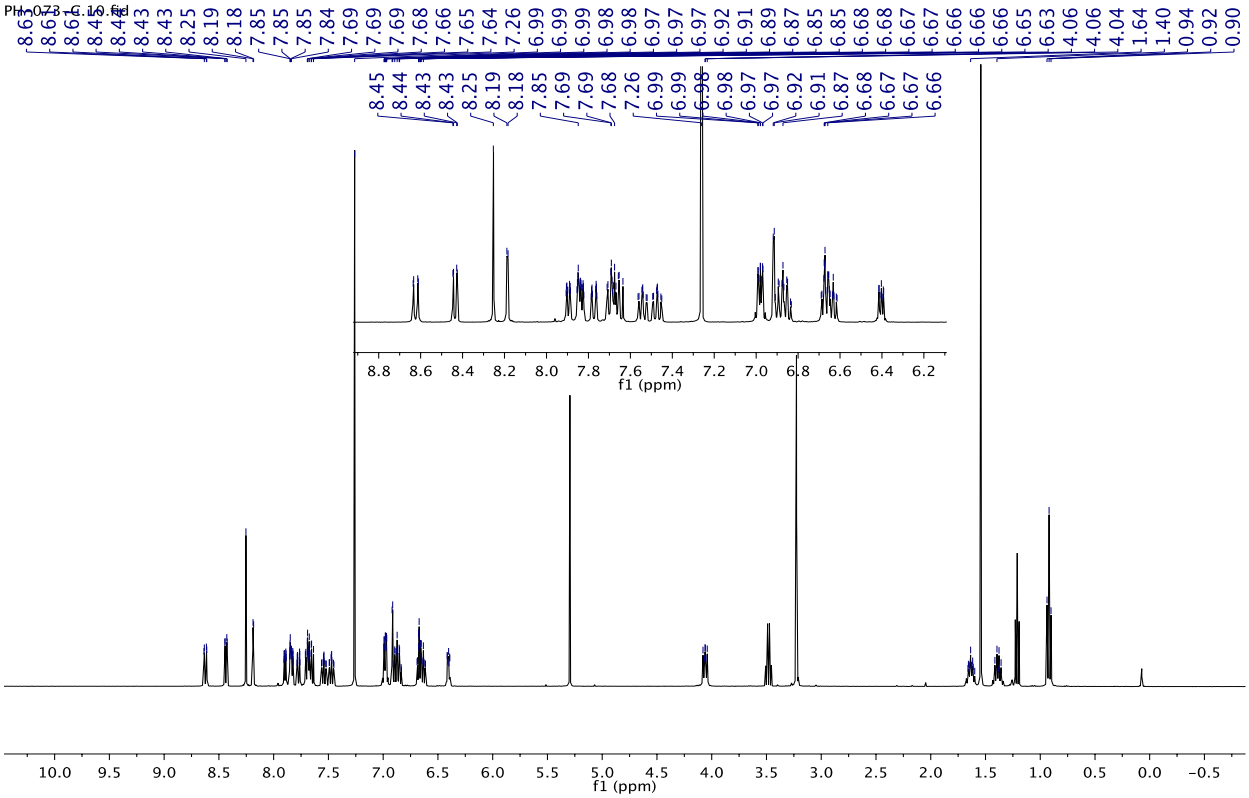


Figure S23.[1]H NMR (400 MHz, $CDCl_3$) of compound **5a**

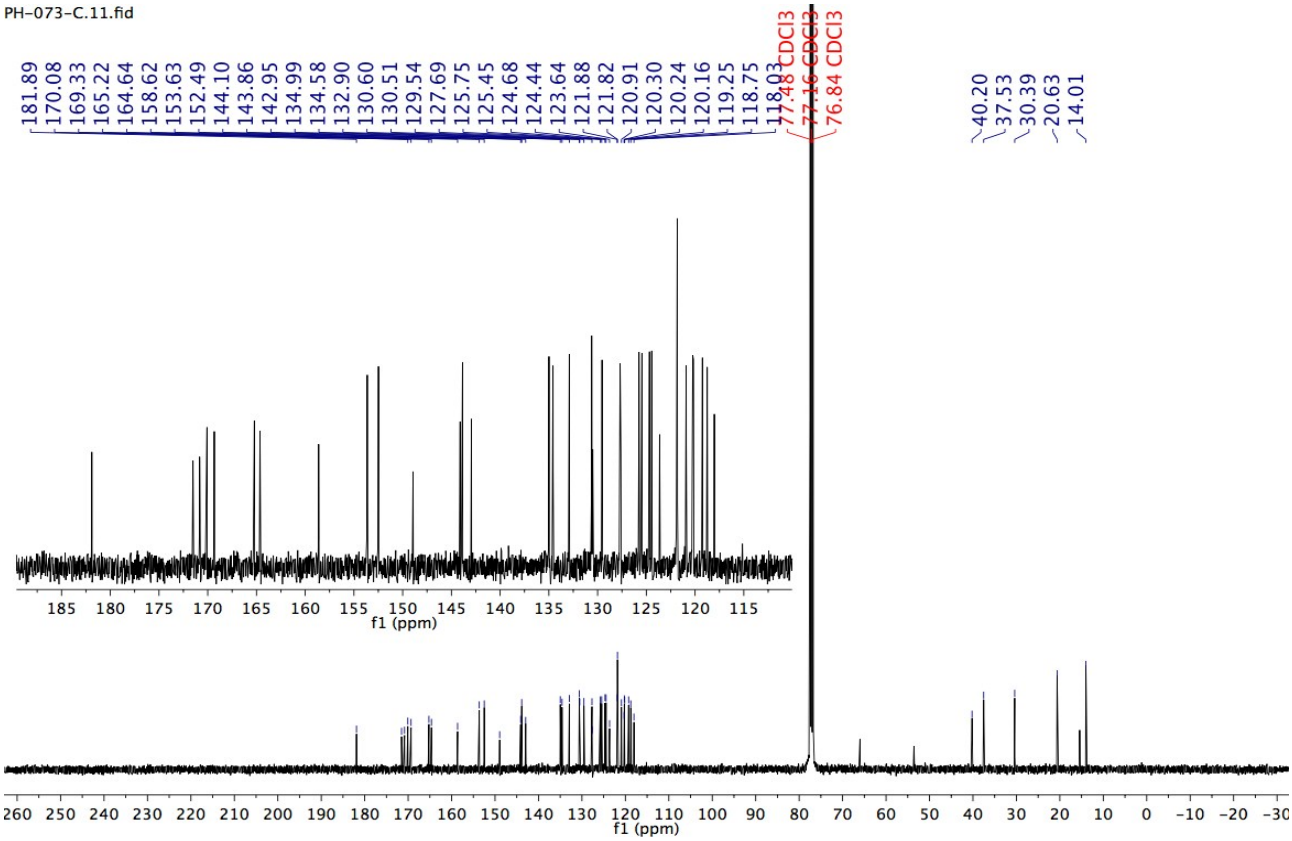


Figure S24. ^{13}C (101 MHz) of compound **5a**

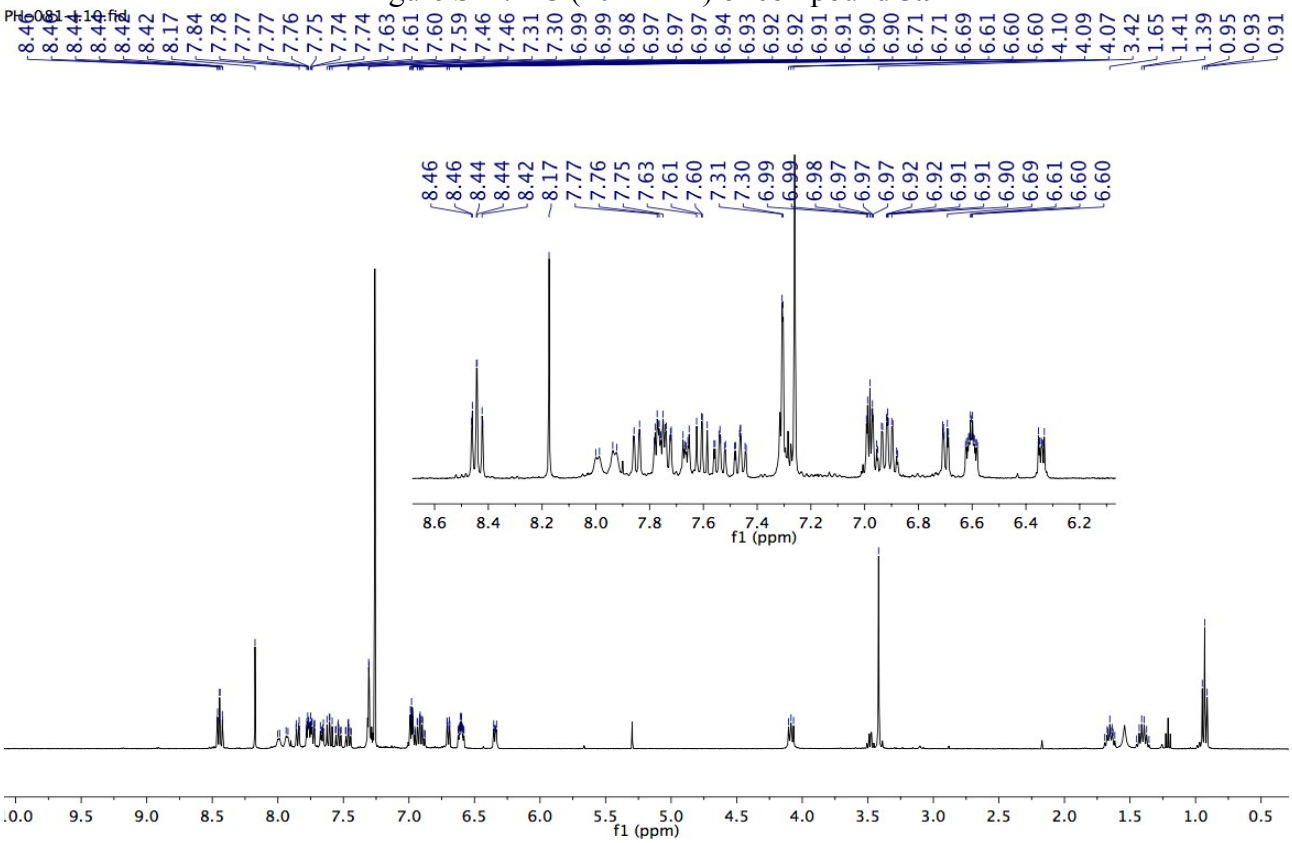


Figure S25.^{1}H NMR (400 MHz) Compound **3b**

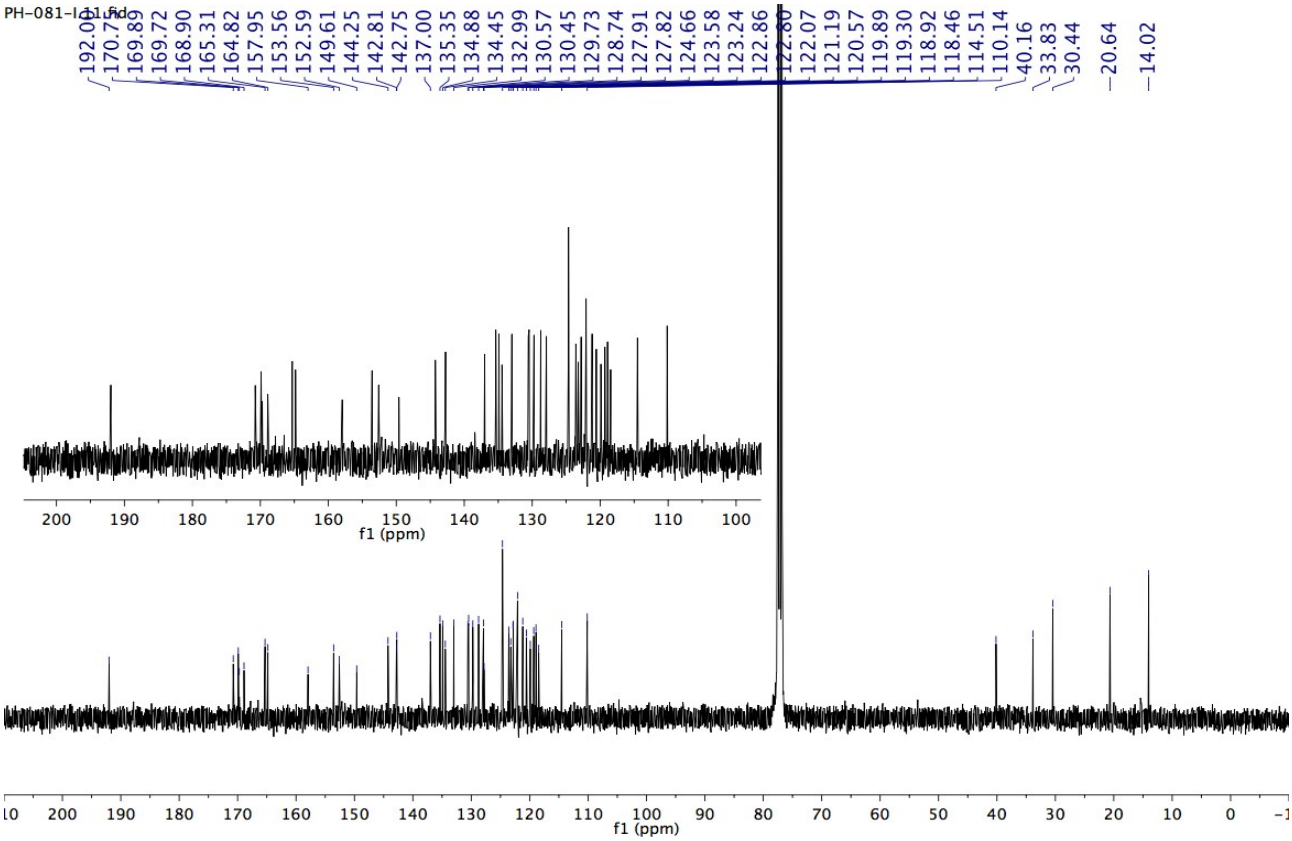


Figure S26.[13]C NMR (101 MHz) Compound **3b**

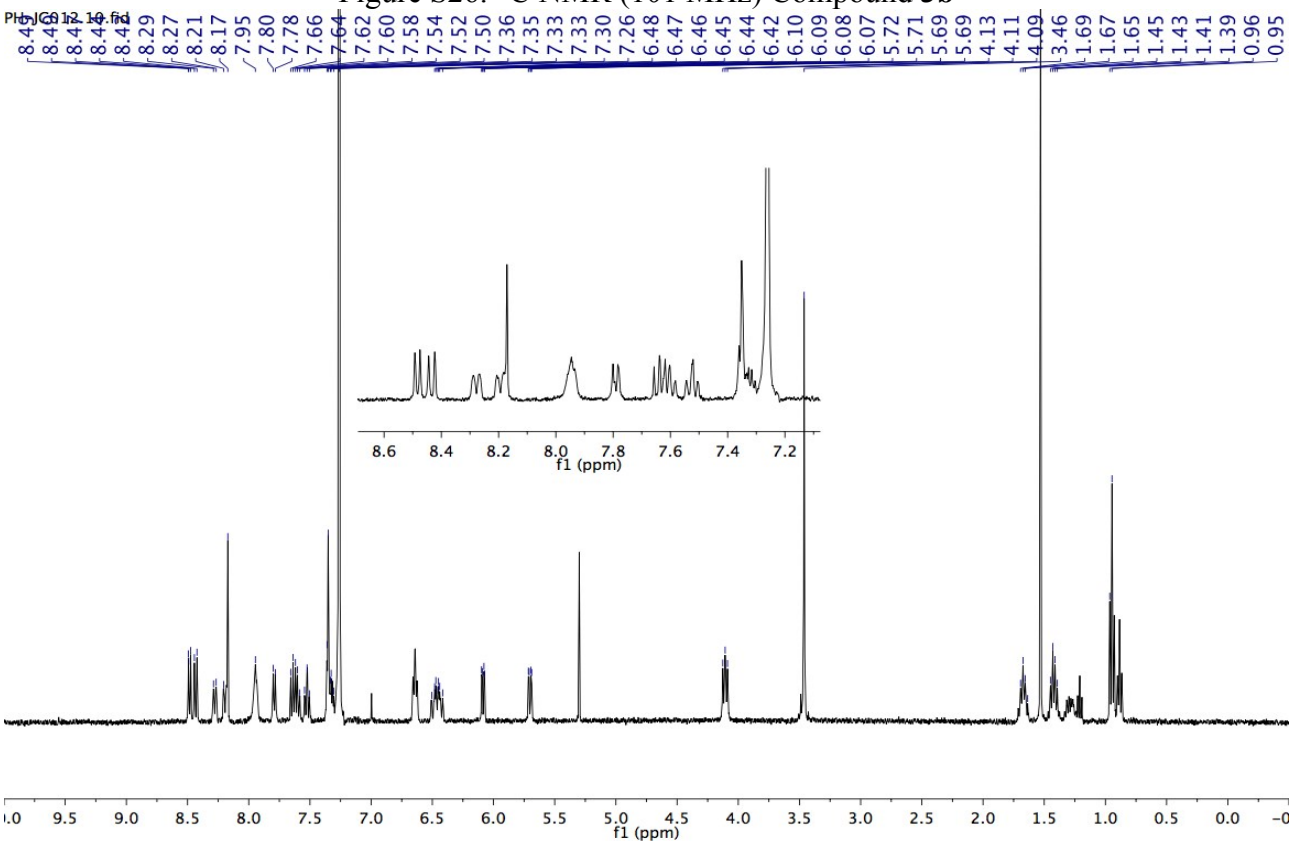


Figure S27.[1]H NMR (400 MHz) Compound **4b**

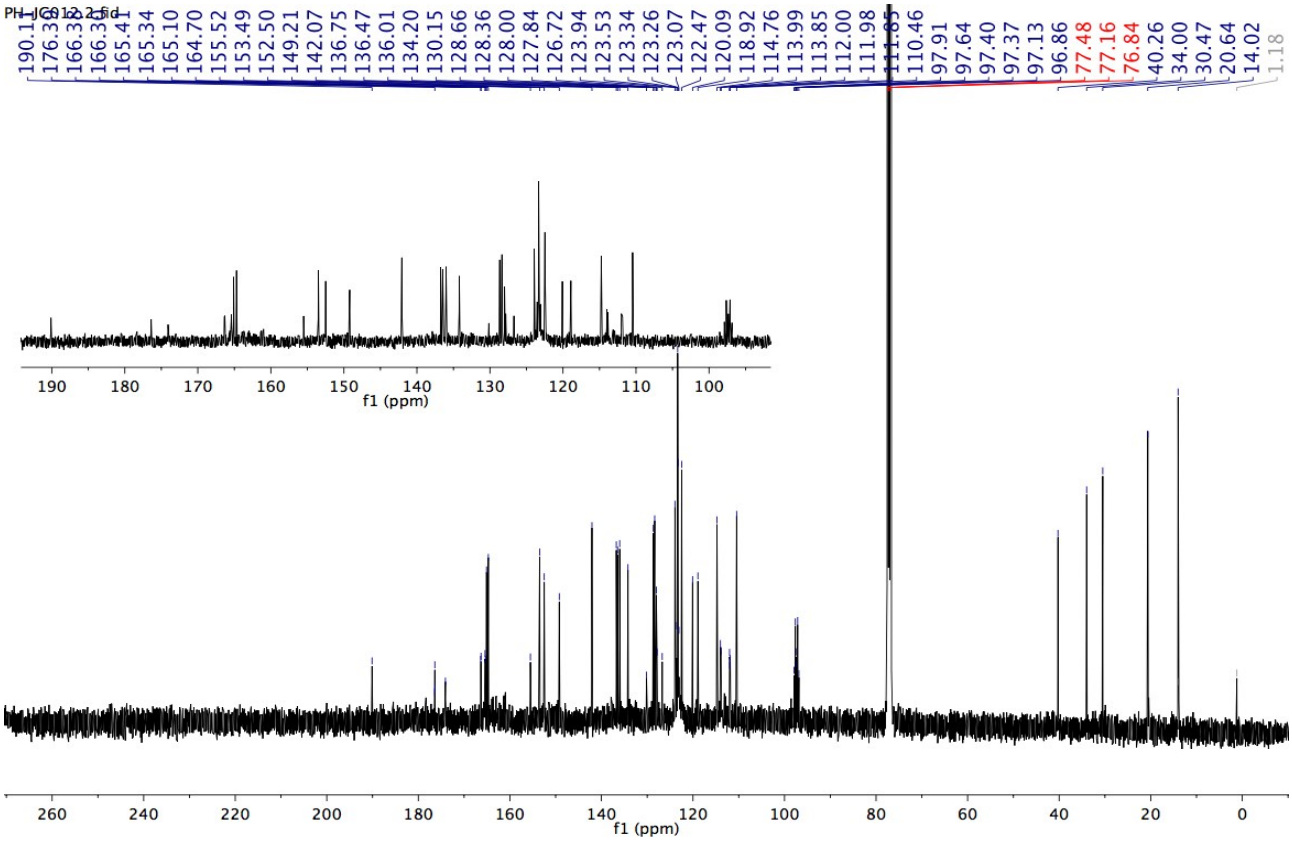


Figure S28.[13]C NMR (101 MHz) Compound **4b**

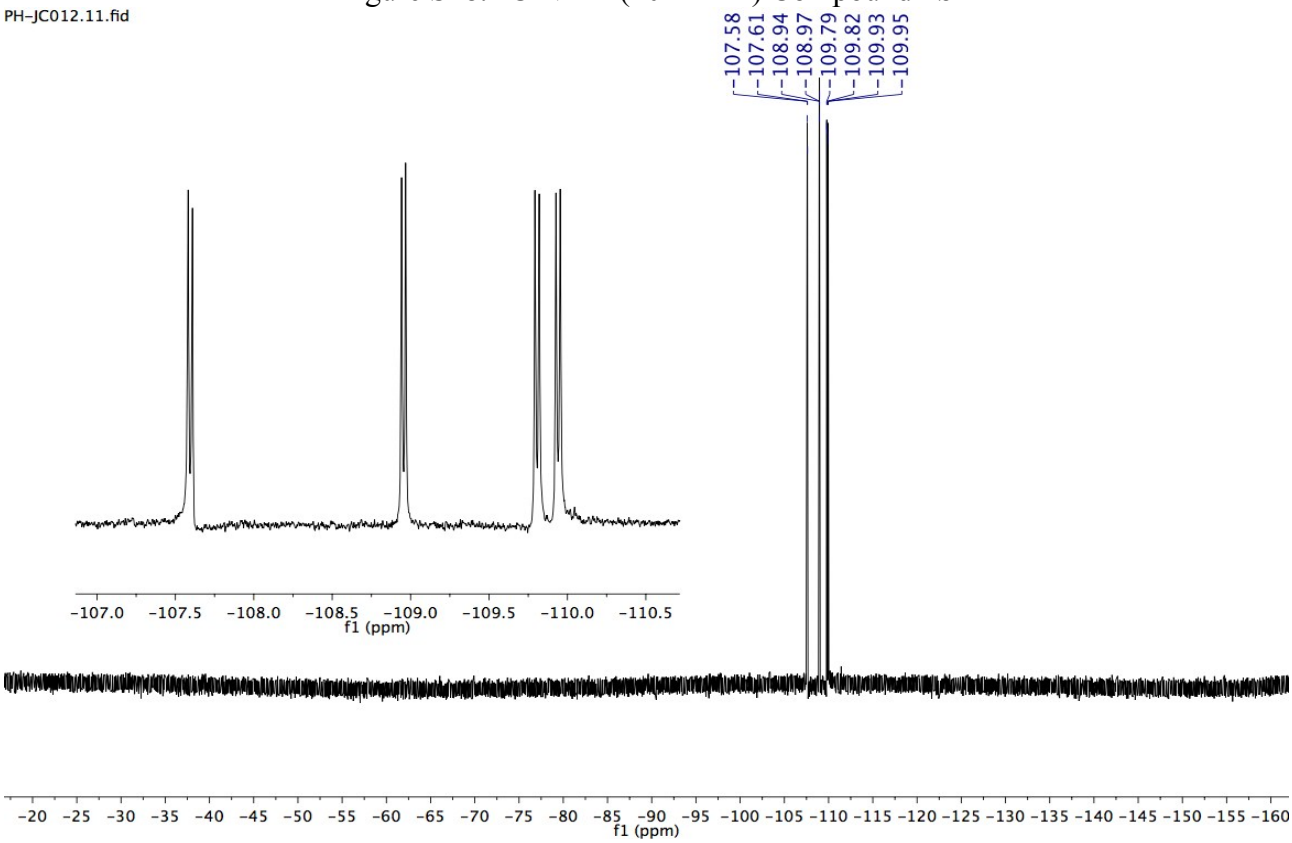


Figure S29.[19]F NMR (376 MHz) Compound **4b**

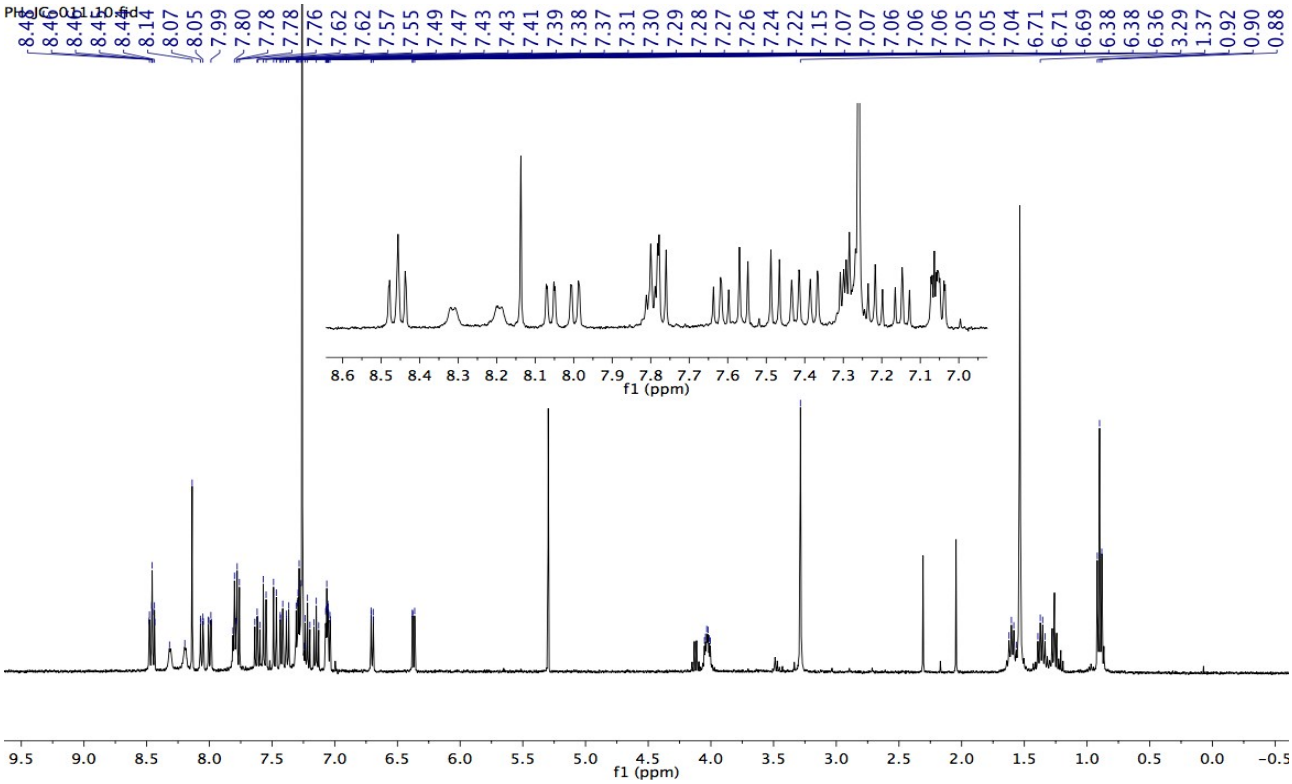


Figure S30.[1]H NMR (400 MHz) Compound **5b**

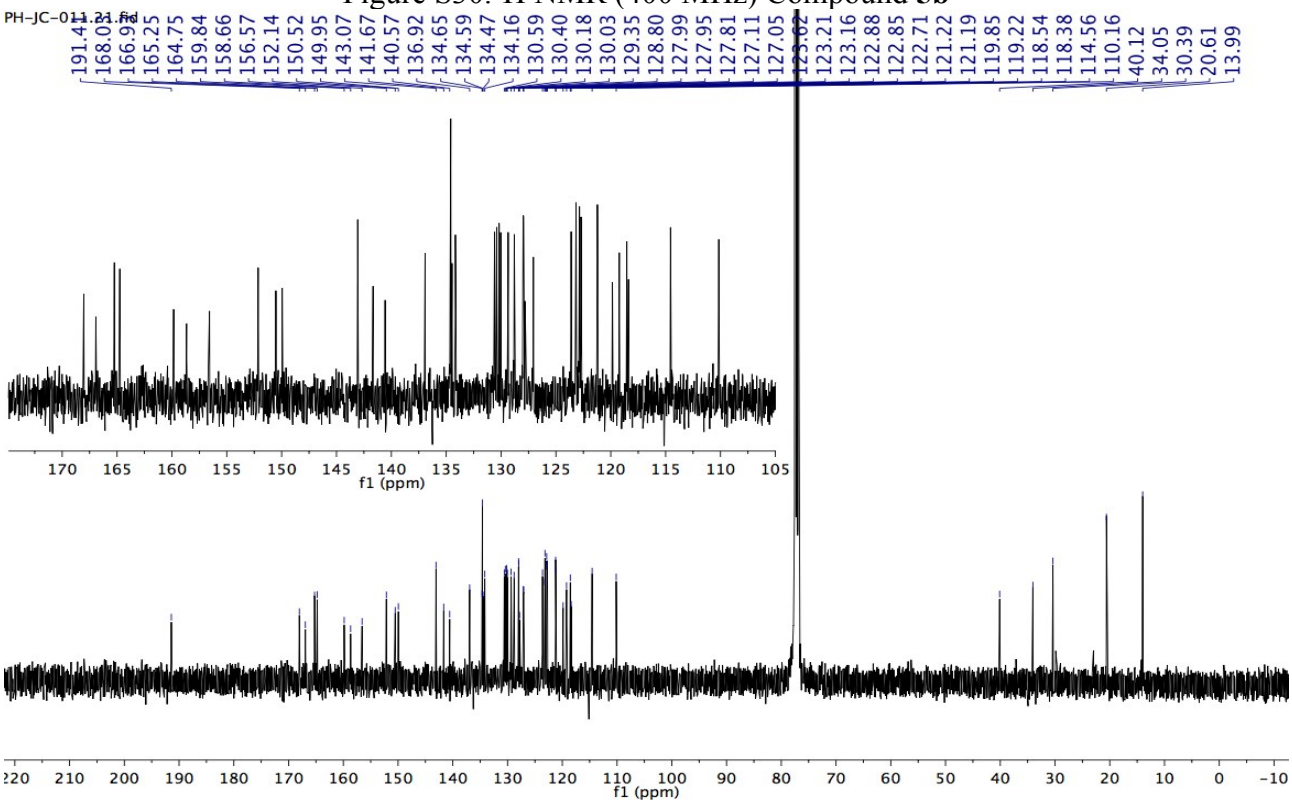


Figure S31. [13]C NMR (101 MHz) Compound **5b**