Cytotoxic Pt(II) complexes containing alizarine:

a selective carrier for DNA metalation

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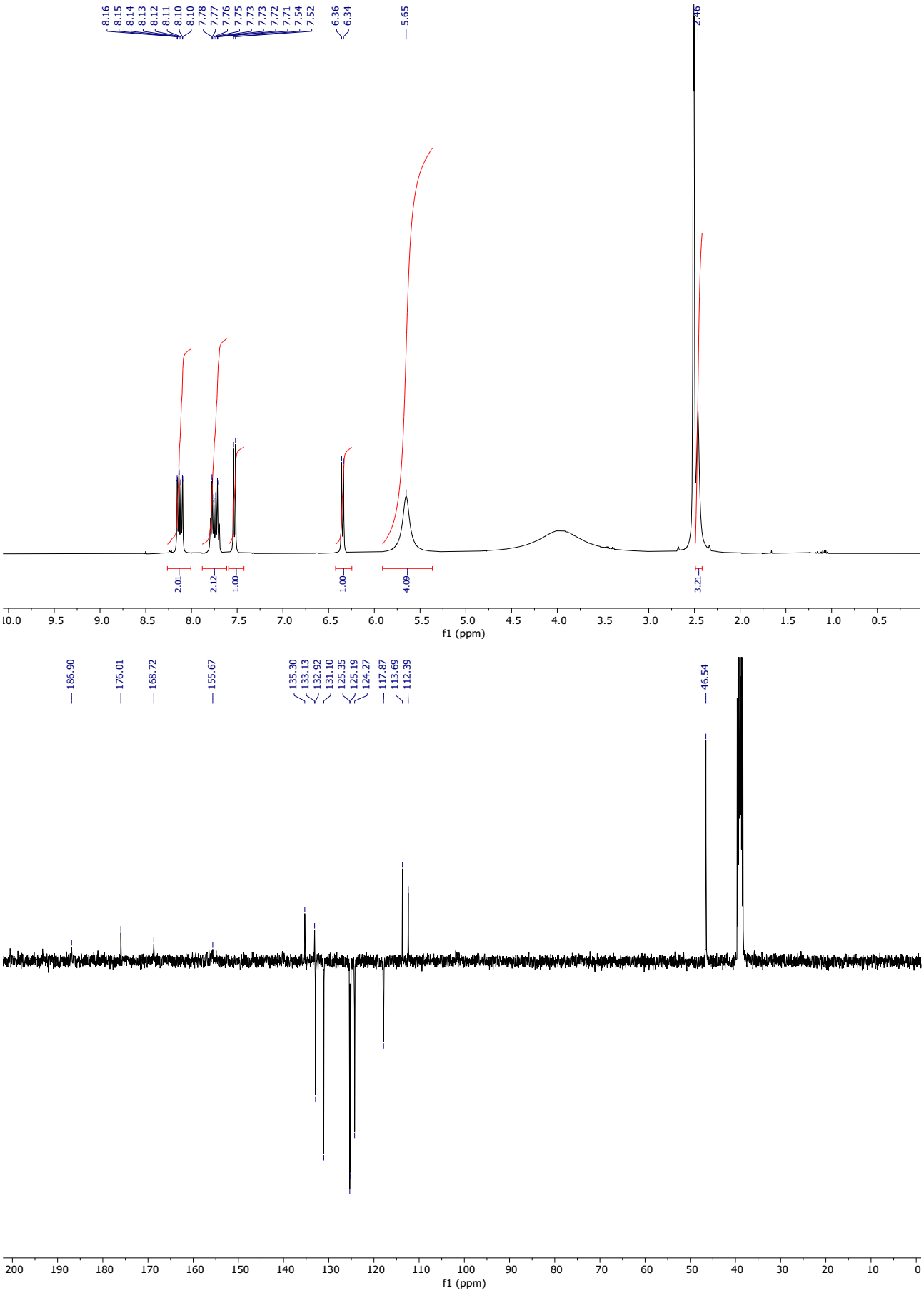


Figure S1. ^{1}H- and ^{13}C-NMR spectra of compound **1b**.

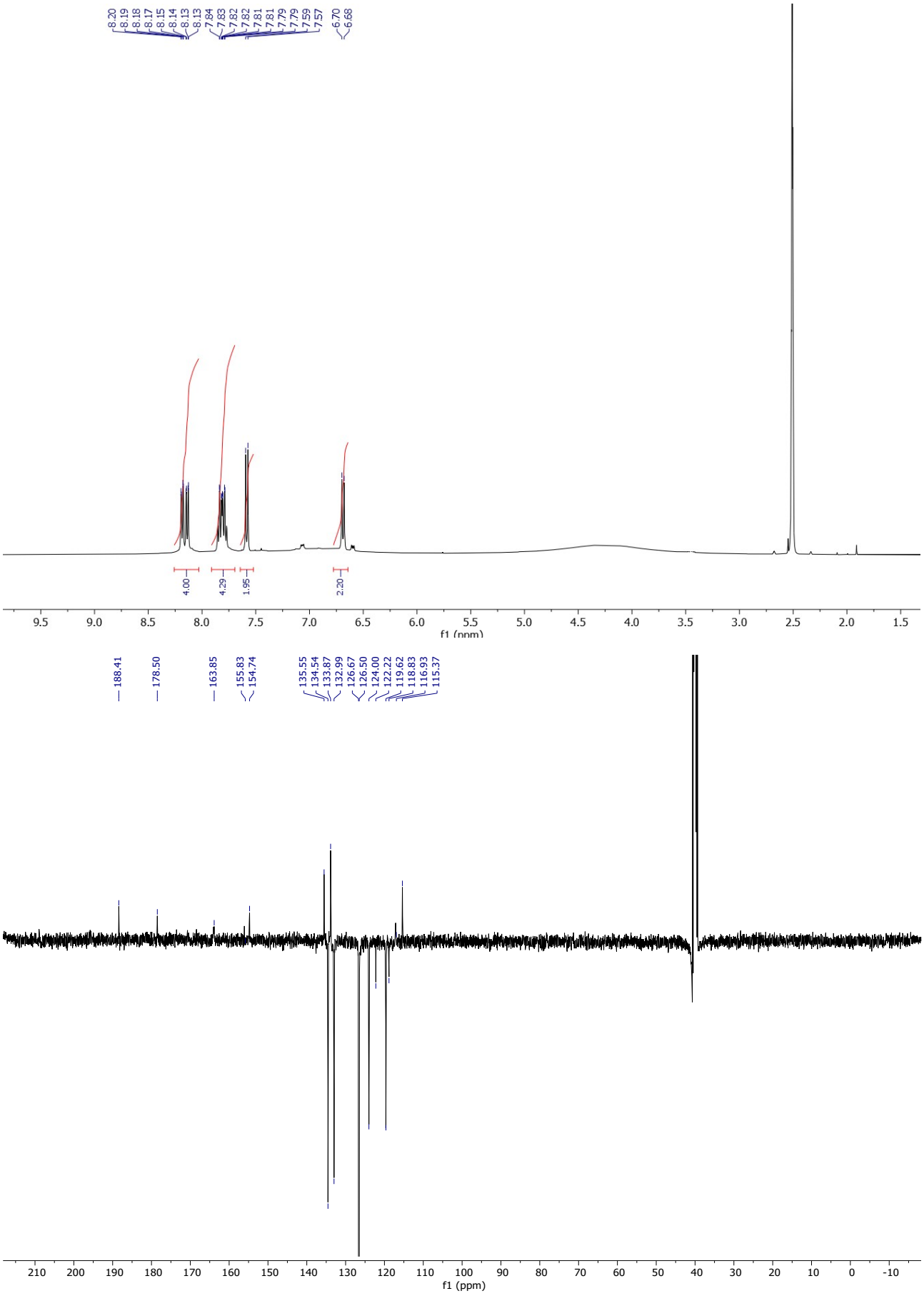


Figure S2. ^{1}H- and ^{13}C-NMR spectra of compound **2b**.

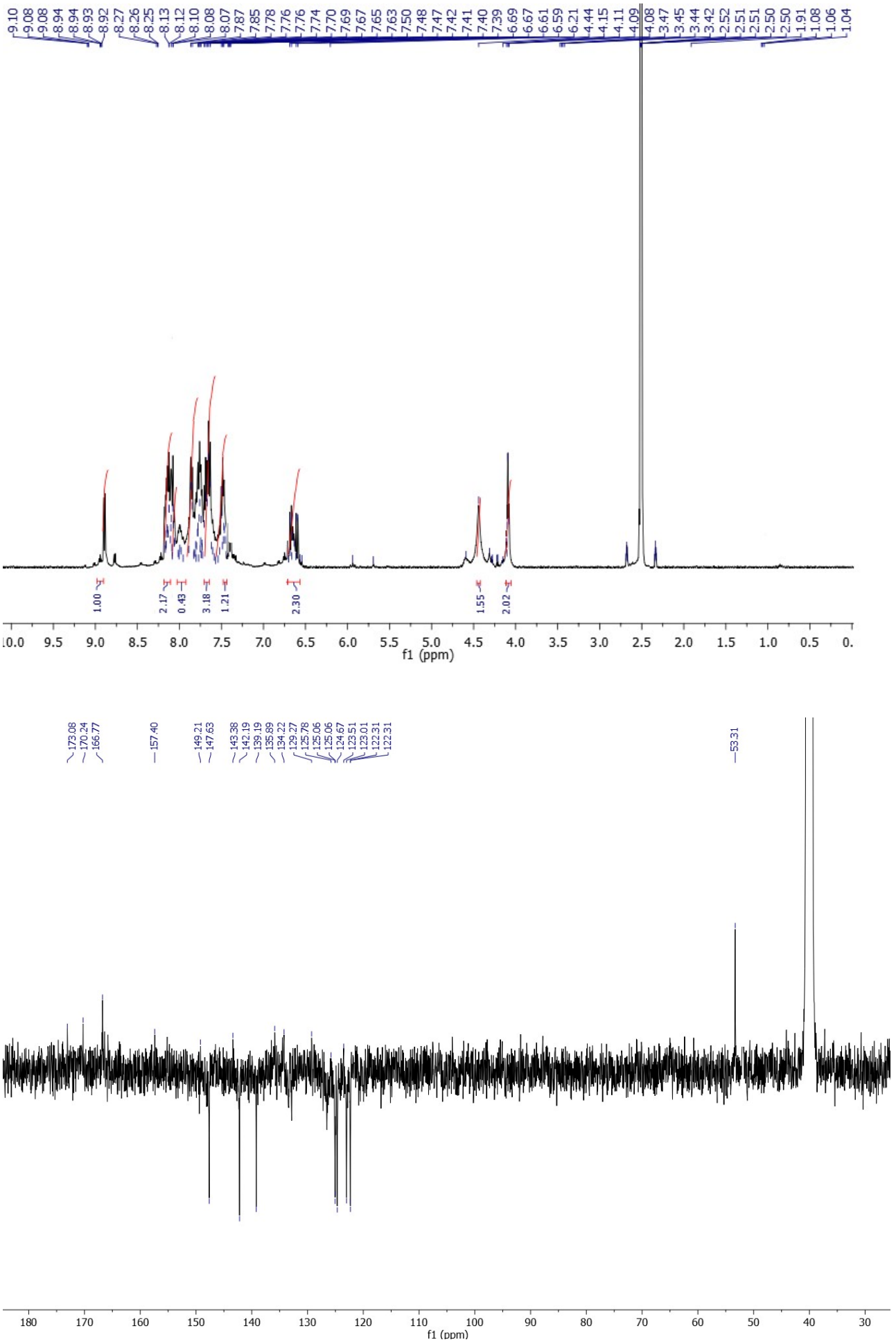


Figure S3. ^{1}H- and ^{13}C-NMR spectra of compound **3b**.

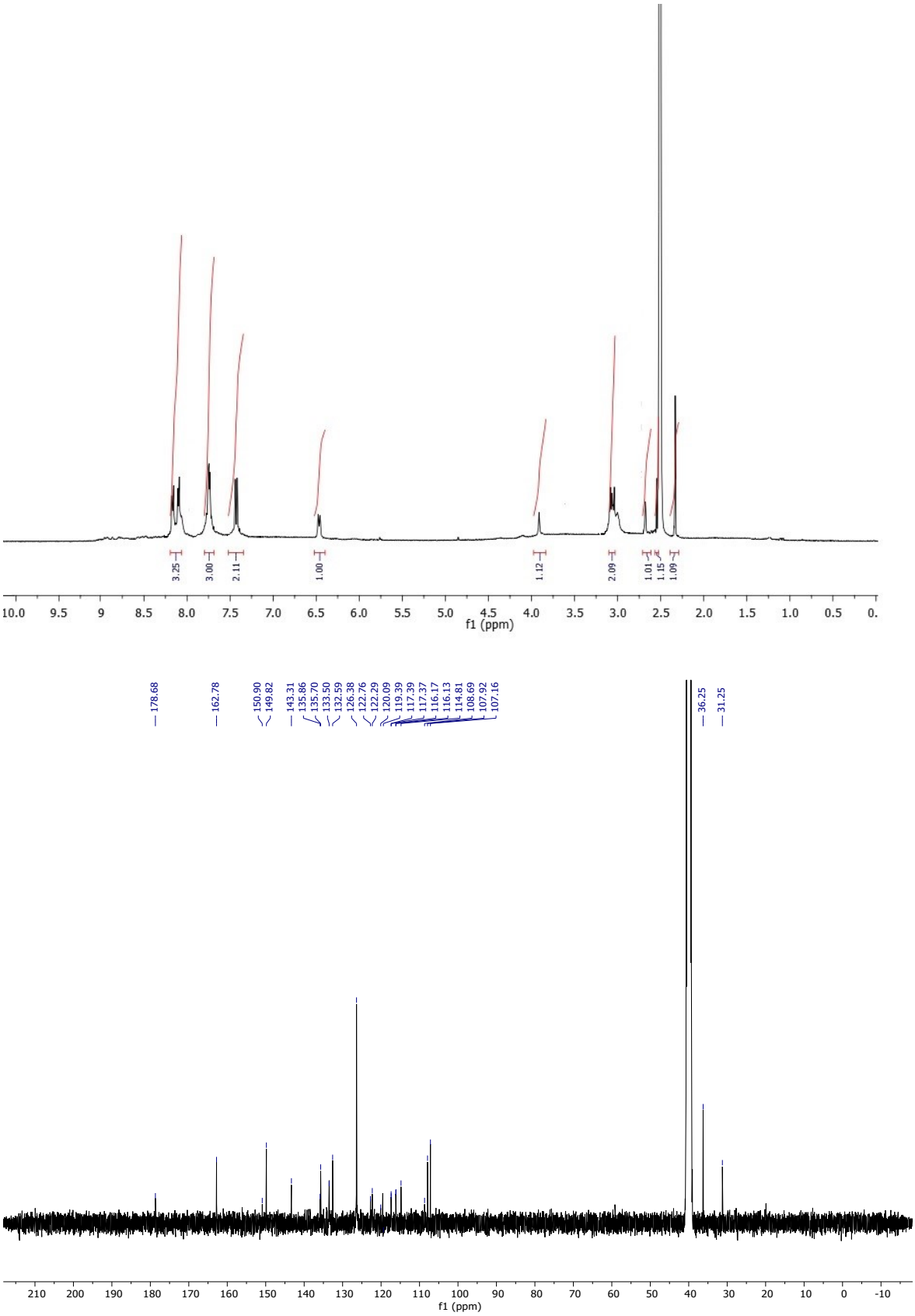


Figure S4. ^{1}H- and ^{13}C-NMR spectra of compound **4b**.

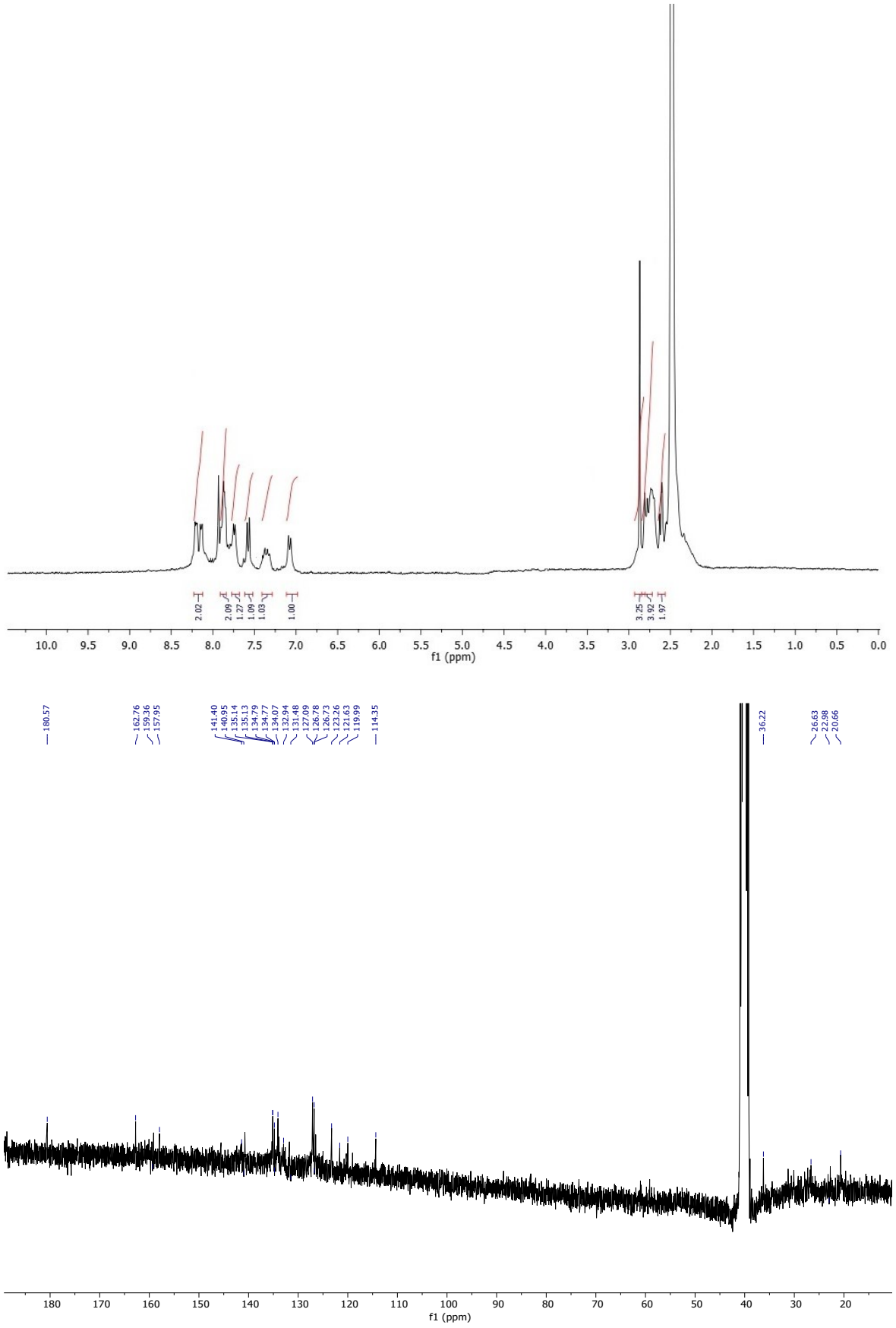


Figure S5. ^{1}H- and ^{13}C-NMR spectra of compound **5b**.

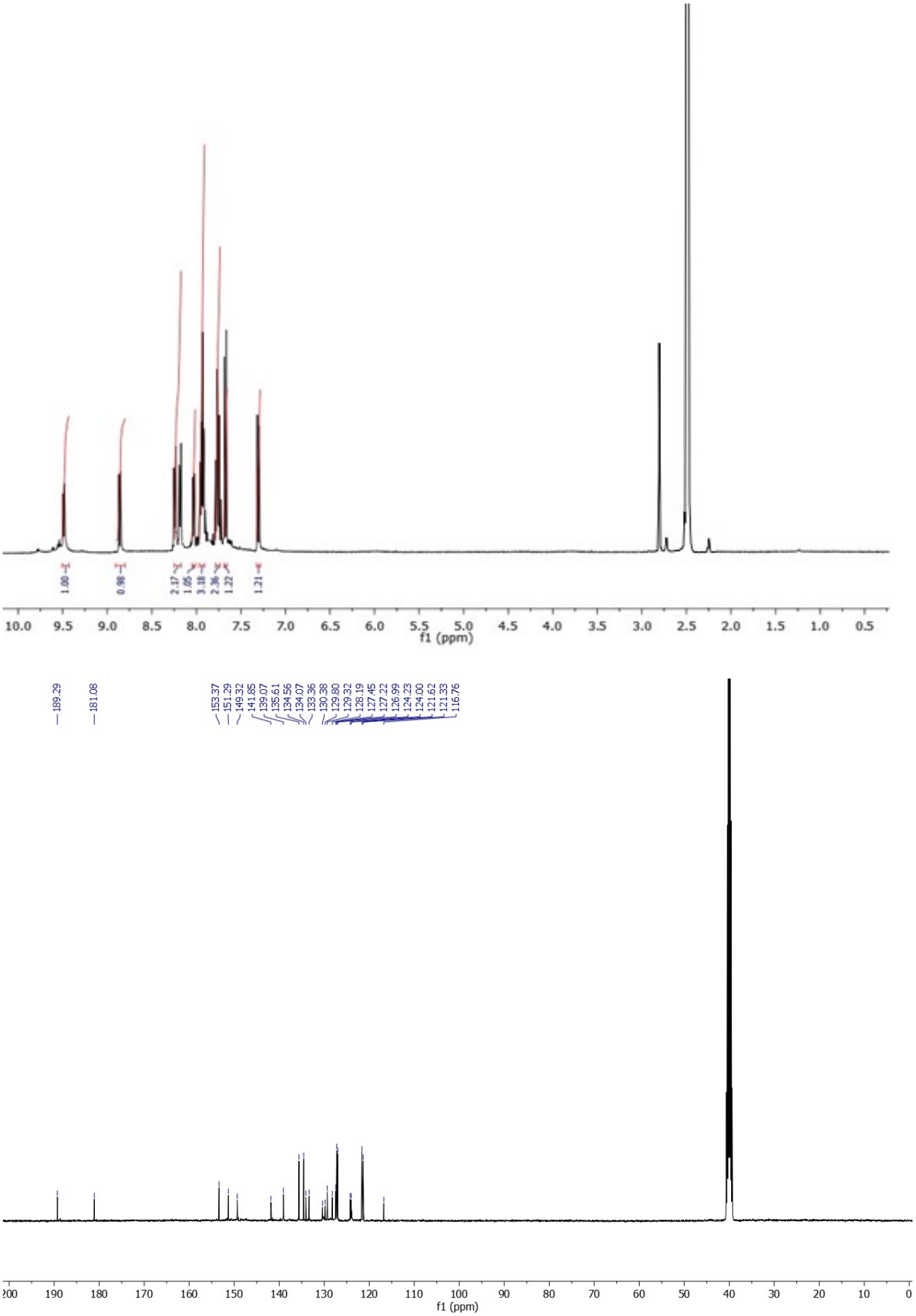


Figure S6. ^{1}H- and ^{13}C-NMR spectra of compound **6b**.

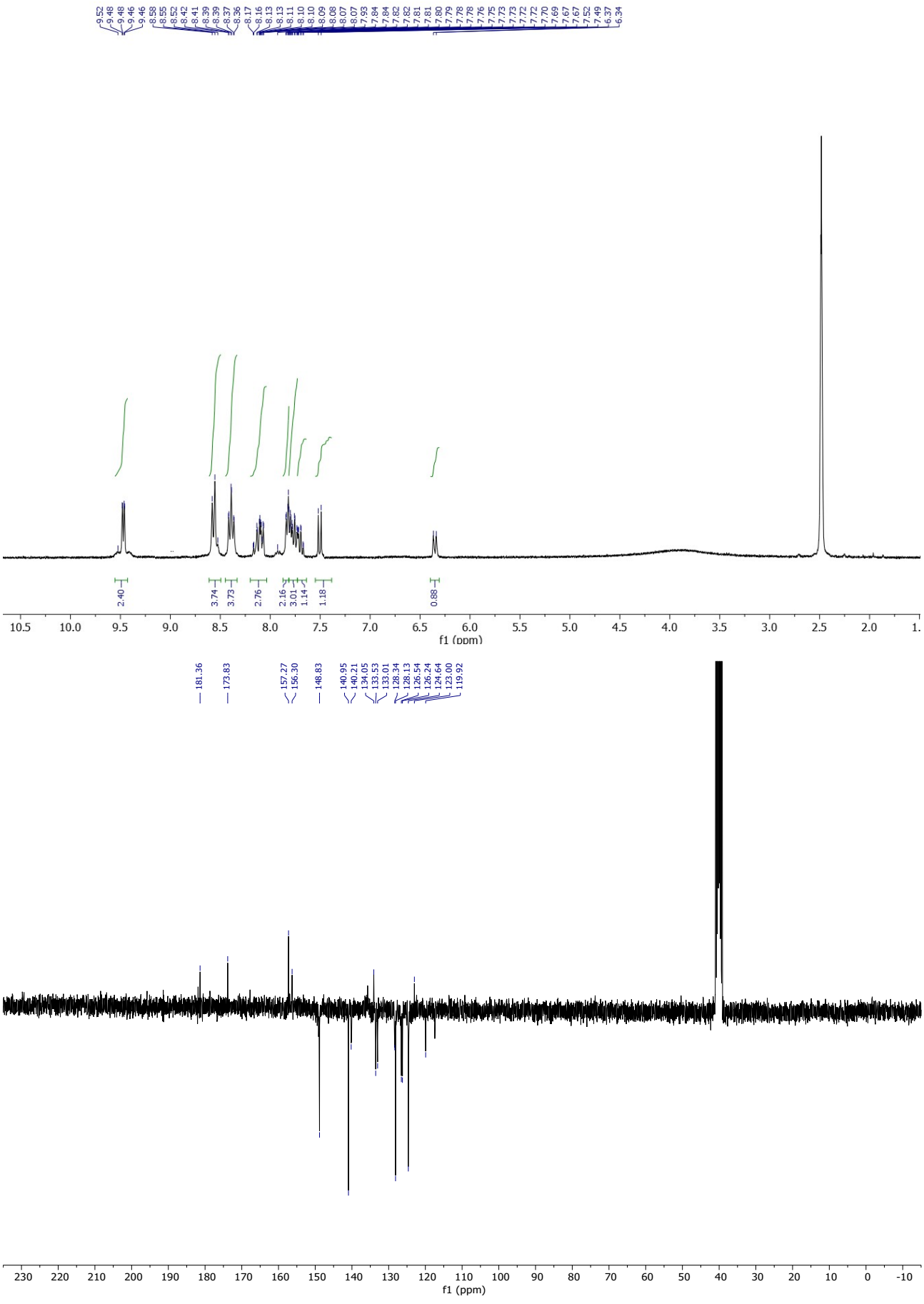


Figure S7. ^{1}H- and ^{13}C-NMR spectra of compound **7b**.

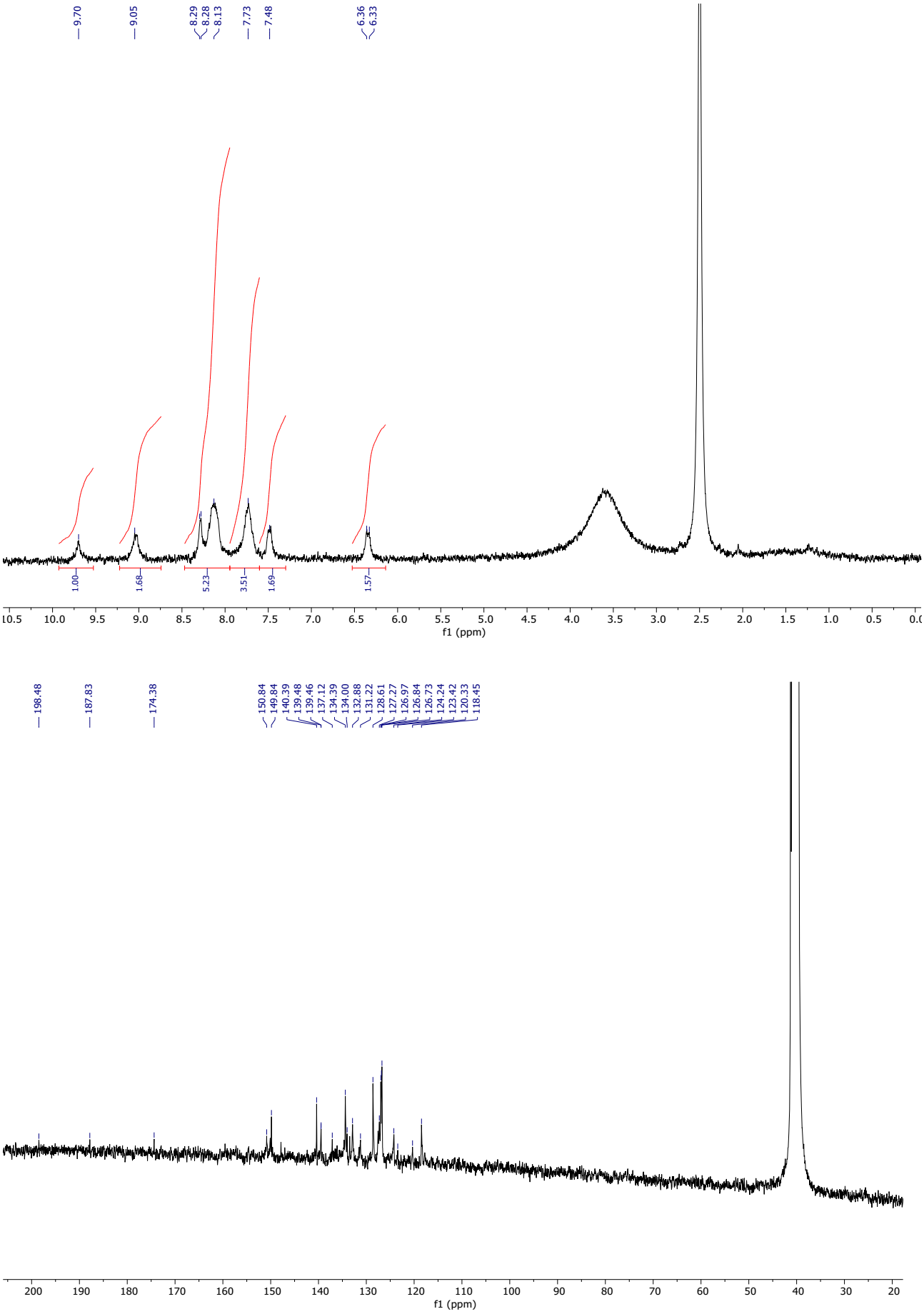


Figure S8. ^{1}H- and ^{13}C-NMR spectra of compound **8b**.

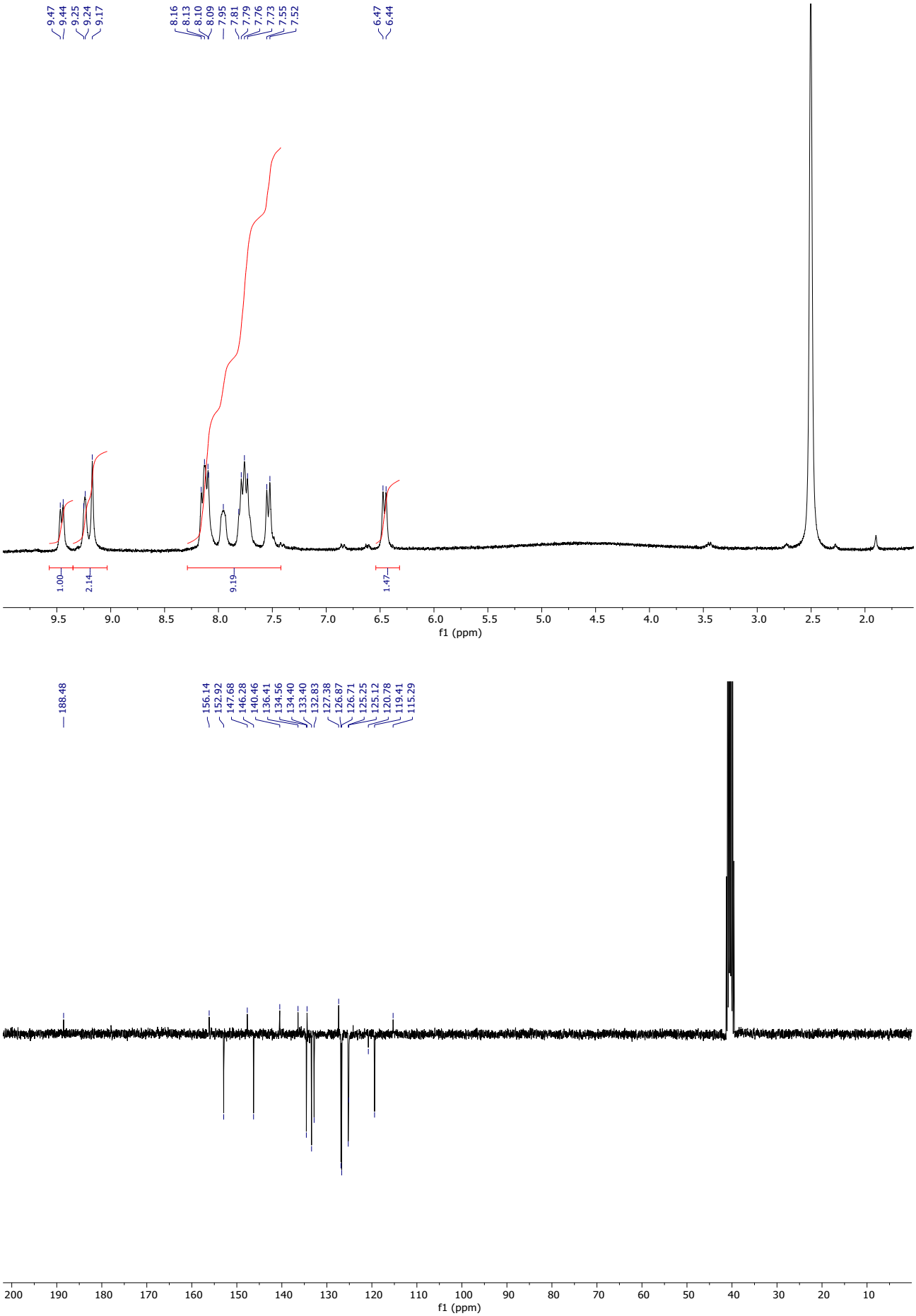


Figure S9. ^{1}H- and ^{13}C-NMR spectra of compound **9b**.

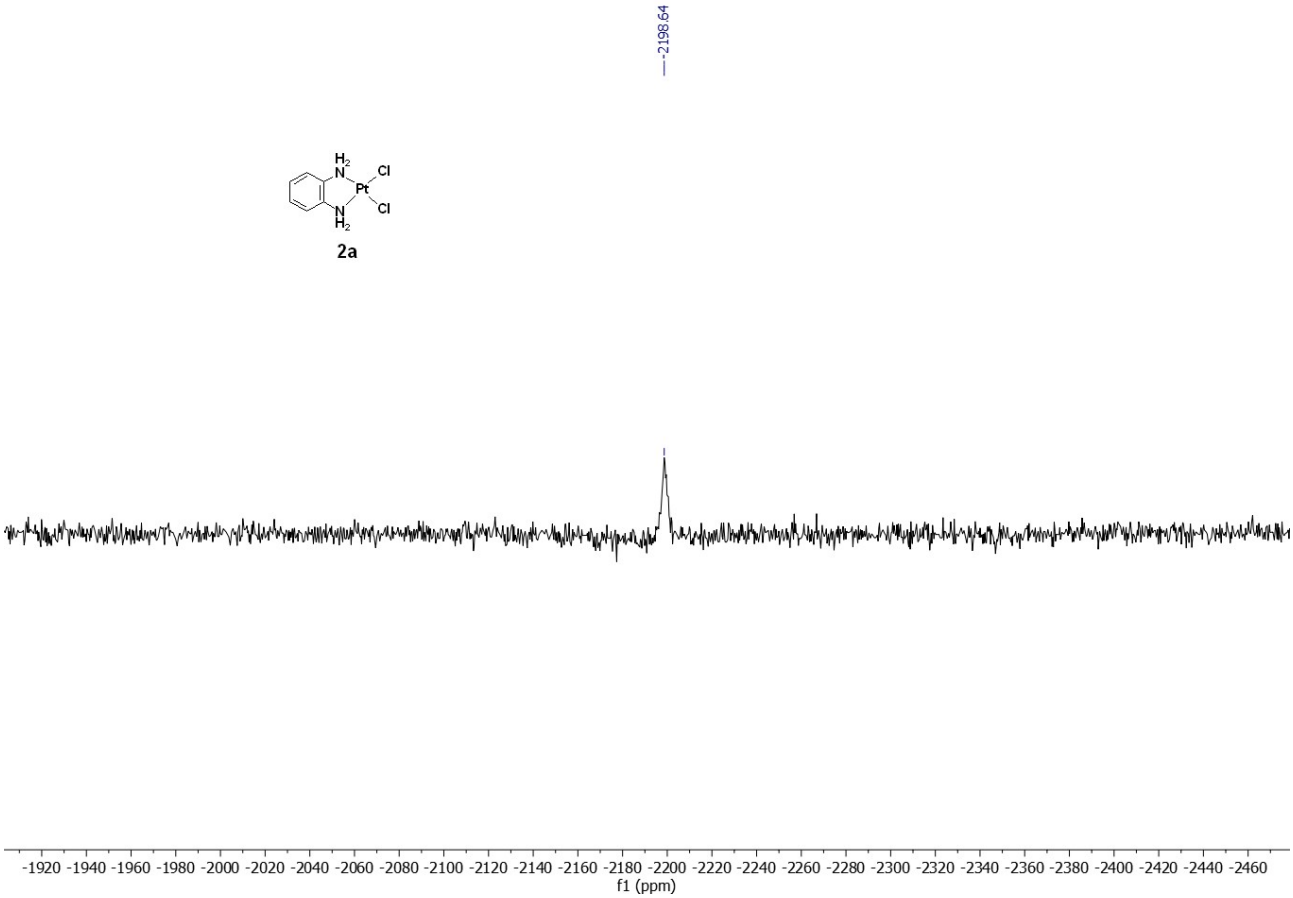


Figure S10. ^{195}Pt-NMR dichloride precursor **2a.**

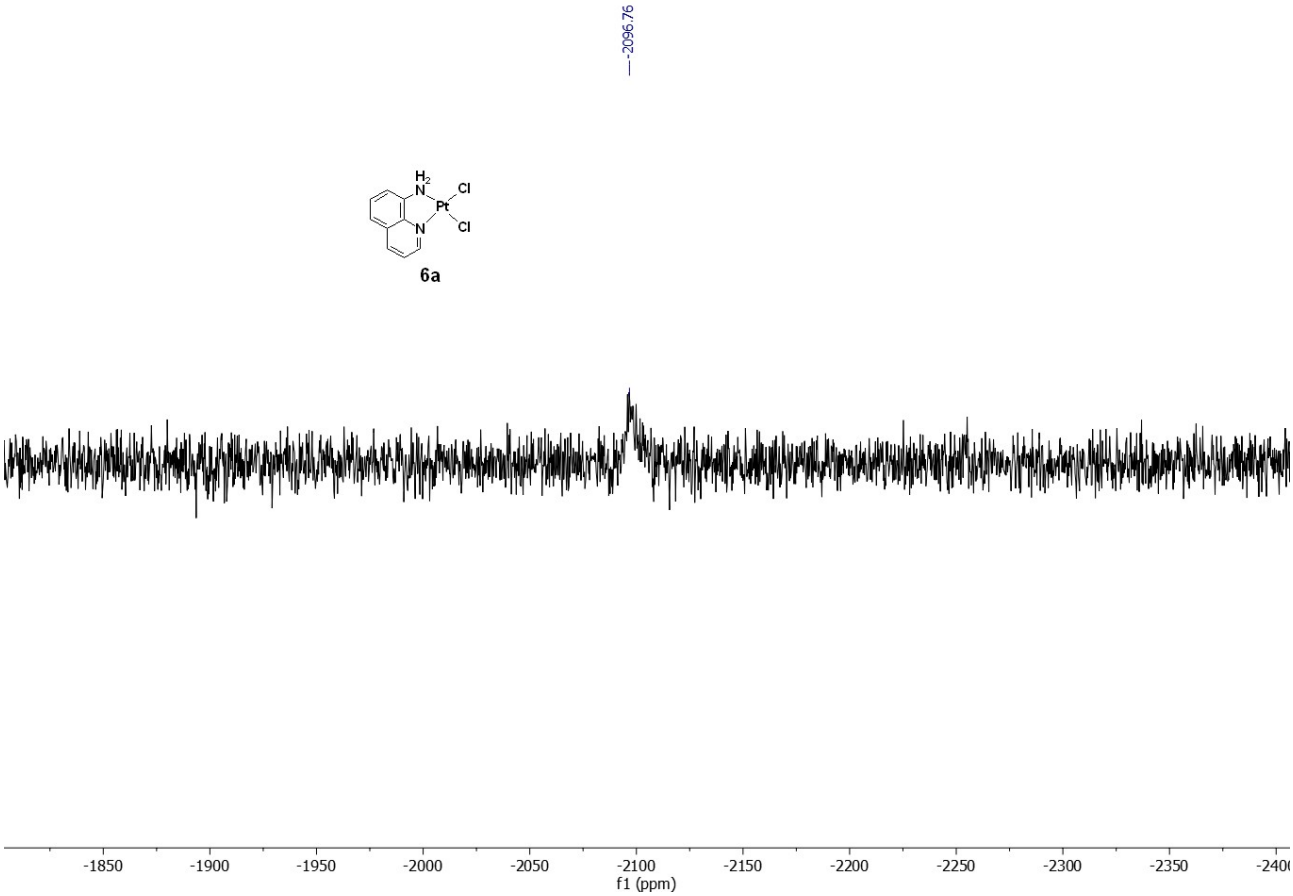


Figure S11. ^{195}Pt-NMR dichloride precursor **6a**.

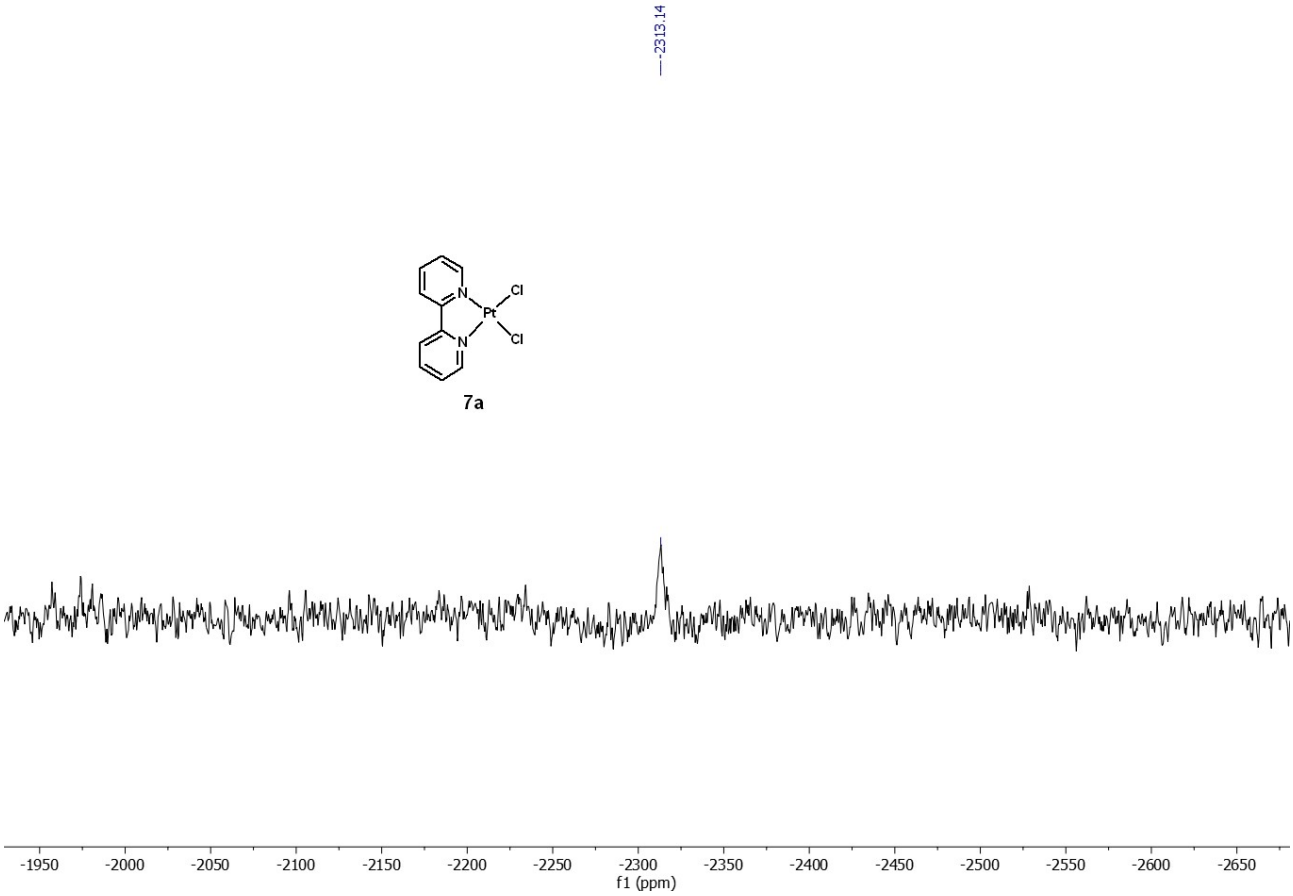
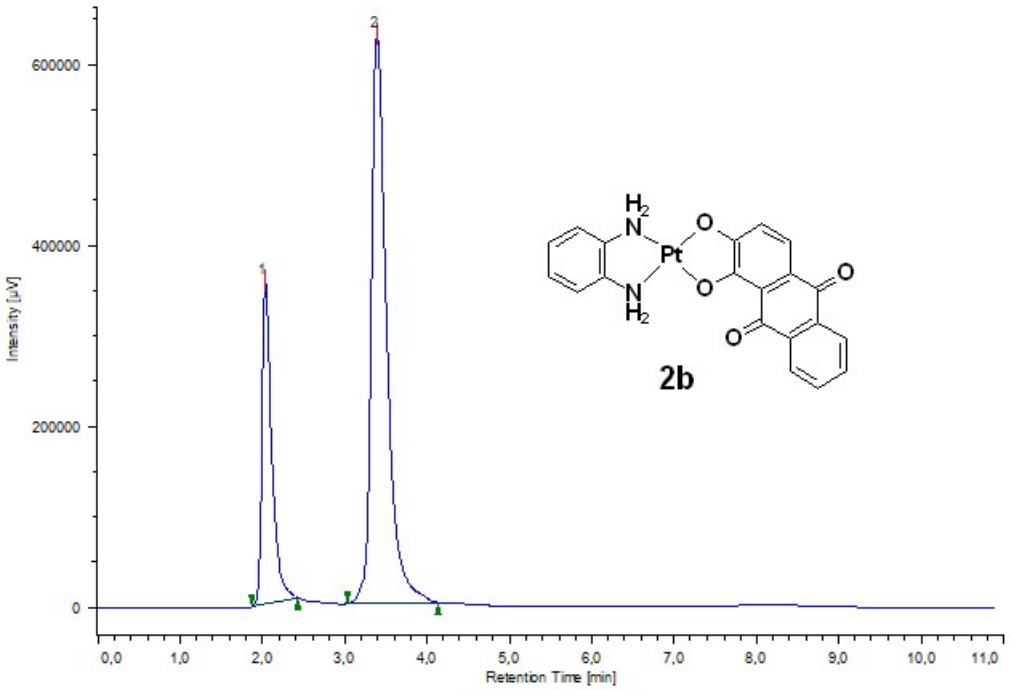
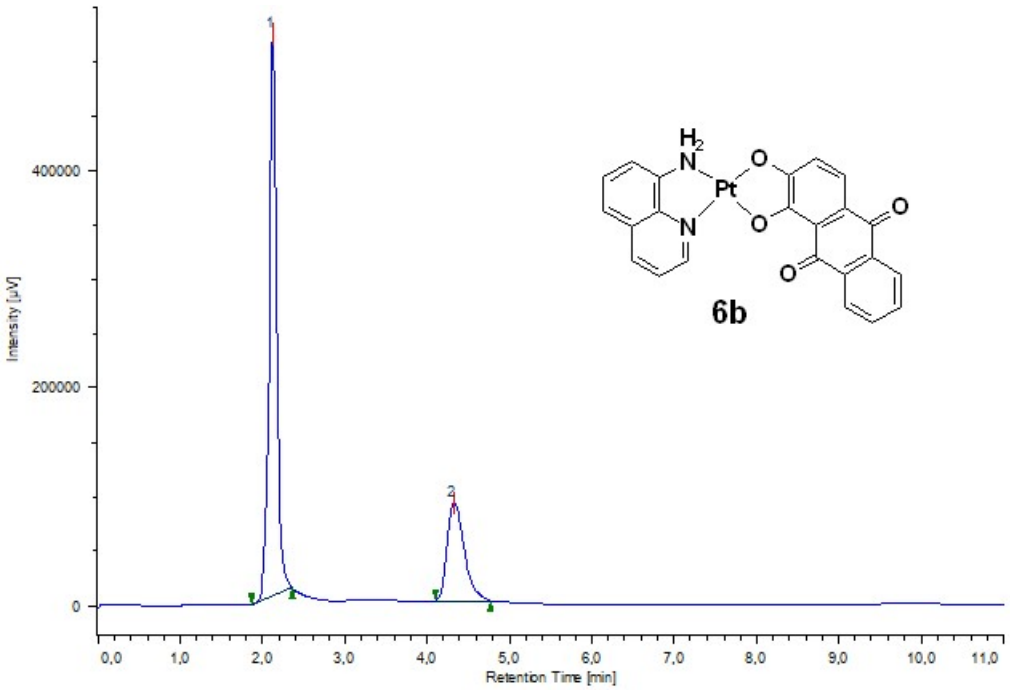


Figure S12. ^{195}Pt-NMR dichloride precursor **7a.**



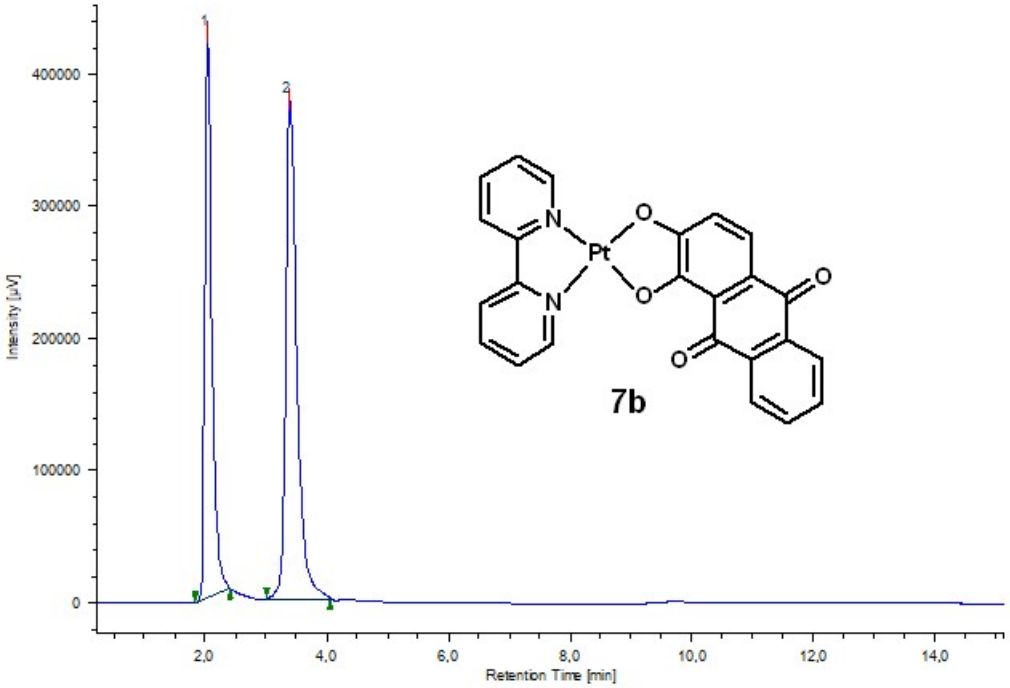
tR	Area	Height	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor
2,033	2984204	356658	26,422	36,249	N/A	1546	5,097	1,678
3,383	8310157	627256	73,578	63,751	N/A	1741	N/A	1,564

Figure S13. HPLC of compound **2b** in presence of KI as internal standard (peak 1).



tR	Area	Height	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor
2,125	3246230	515045	71,234	85,207	N/A	3315	8,313	1,021
4,325	1310879	89420	28,766	14,793	N/A	2040	N/A	1,363

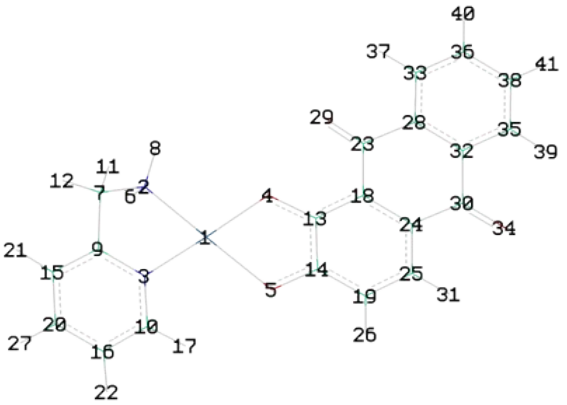
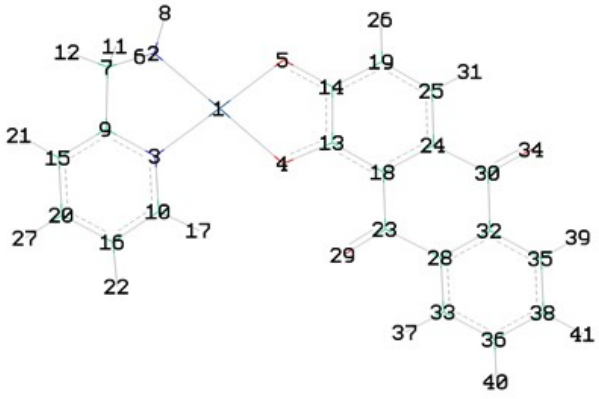
Figure S14. HPLC of compound **6b** in presence of KI as internal standard (peak 1).



tR	Area	Height	Area%	Height%	Quantity	NTP	Resolution	Symmetry Factor
2,042	3459561	426282	41,796	53,098	N/A	1694	5,282	1,524
3,392	4817710	376543	58,204	46,902	N/A	1866	N/A	1,522

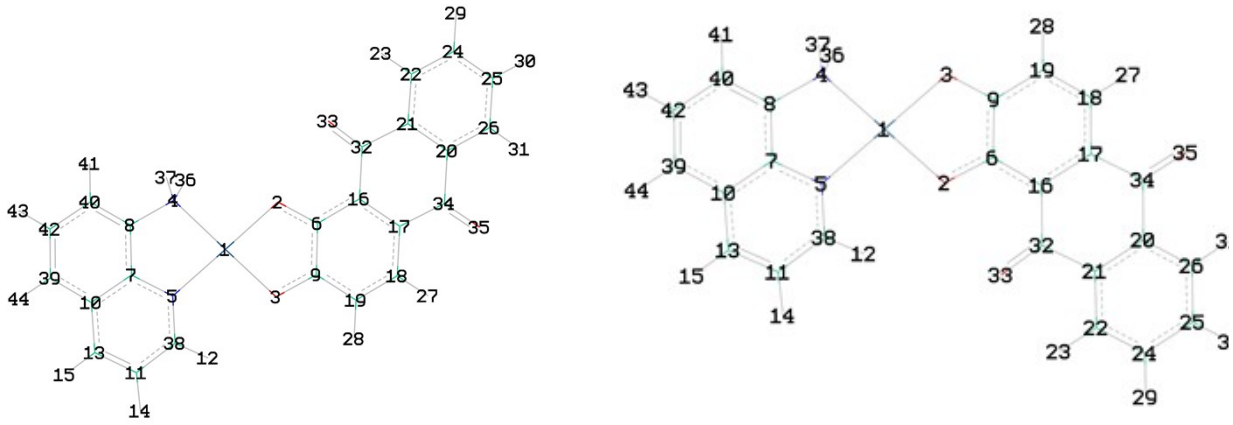
Figure S15. HPLC of compound **7b** in presence of KI as internal standard (peak 1).

Table TS1. ^{1}H and ^{13}C chemical shift (*δ, ppm*) computed in DMSO for the two possible isomers of complexes **3b**-**6b**.

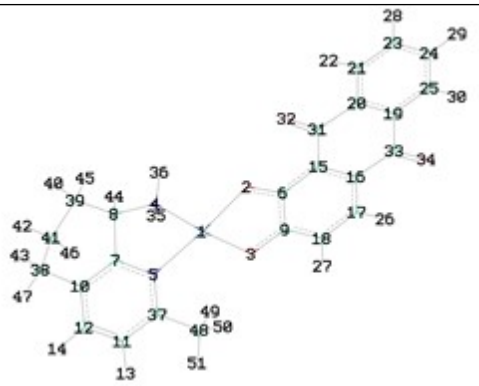
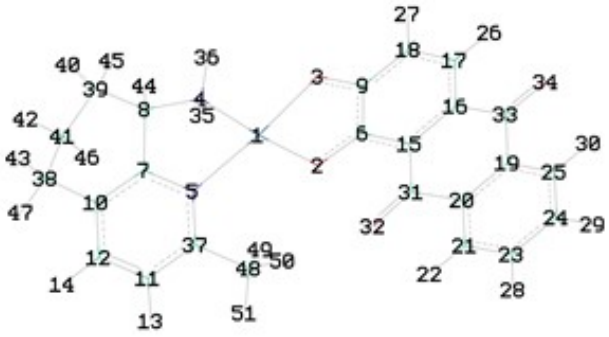
		cis		*trans*	
3b					
		Label	*δ (ppm)*	*Label*	*δ (ppm)*
^{1}H		H17	9.40	H17	9.79
		H37	9.09	H37	9.14
		H39	9.00	H39	9.01
		H27	8.64	H27	8.66
		H31	8.47	H40	8.48
		H40	8.46	H31	8.46
		H41	8.44	H41	8.44
		H21	8.24	H21	8.25
		H22	8.22	H22	8.33
		H26	7.49	H26	7.49
		H11	5.05	H11	5.03

	H12	4.97	H12	4.95
	H6	4.36	H6	4.23
	H8	4.29	H8	4.09
^{13}C	C23	204.78	C23	204.97
	C30	202.01	C30	202.41
	C14	192.84	C14	193.18
	C13	187.16	C13	184.93
	C9	179.27	C9	179.25
	C10	168.85	C10	168.73
	C20	157.96	C20	157.61
	C28	152.79	C28	152.80
	C36	151.50	C36	151.72
	C32	151.40	C32	151.36
	C38	151.00	C38	151.11
	C33	144.94	C33	145.05
	C35	144.42	C35	144.50
	C16	143.58	C16	143.53
	C15	141.08	C15	140.94
	C24	140.18	C24	140.50
	C25	139.39	C25	139.24
	C18	136.87	C18	136.40
	C19	133.46	C19	134.70
	C7	66.52	C7	66.15

4b

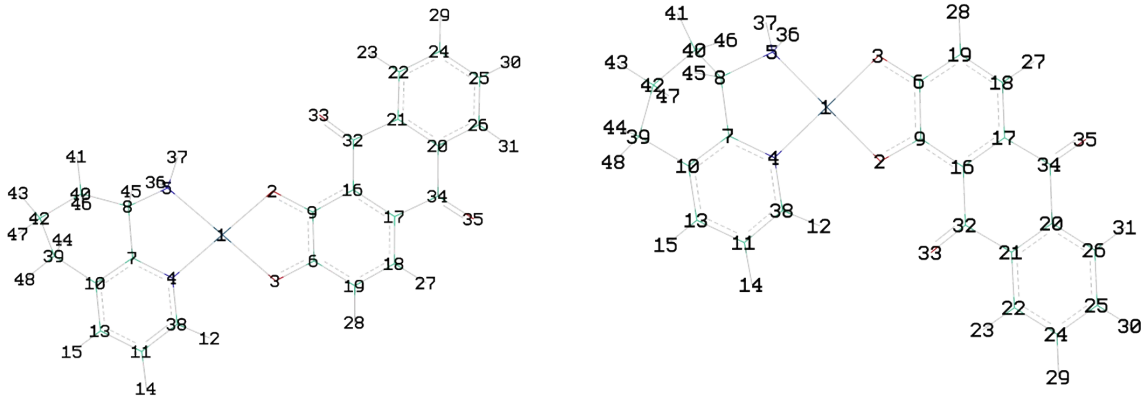


	Label	*δ (ppm)*	*Label*	*δ (ppm)*
^{1}H	H12	10.29	H12	10.00
	H15	9.21	H15	9.19
	H23	9.21	H23	9.16
	H31	9.05	H31	9.04
	H44	8.91	H44	8.91
	H41	8.84	H41	8.87
	H43	8.65	H43	8.66
	H14	8.57	H29	8.52
	H29	8.54	H14	8.49
	H30	8.49	H30	8.48
	H27	8.41	H27	8.44
	H28	7.55	H28	7.60
	H36	6.29	H37	6.40
	H37	6.27	H36	6.38
^{13}C	C32	184.99	C32	185.93
	C34	182.61	C34	183.88
	C9	170.65	C9	170.38
	C6	164.97	C6	166.45
	C38	148.68	C38	148.39
	C7	143.43	C7	143.36
	C13	138.89	C13	138.90
	C21	133.97	C21	133.77
	C8	133.53	C8	133.58

	C20	132.72	C20	132.62
	C24	131.63	C24	131.66
	C25	131.12	C25	131.19
	C39	129.58	C39	129.59
	C10	129.02	C10	128.94
	C40	128.59	C40	128.47
	C42	128.08	C42	128.17
	C22	126.49	C22	126.51
	C26	126.10	C26	126.27
	C17	123.35	C17	122.85
	C11	123.07	C11	122.91
	C18	122.63	C18	123.21
	C16	120.90	C16	120.86
	C19	117.61	C19	117.10
5b				
	Label	*δ (ppm)*	*Label*	*δ (ppm)*
^{1}H	H22	9.02	H22	9.11
	H30	8.94	H30	9.00
	H26	8.42	H28	8.46
	H28	8.41	H26	8.46
	H29	8.38	H29	8.43
	H14	8.30	H14	8.37
	H13	8.01	H13	8.15
	H27	7.39	H27	7.50
	H44	5.03	H44	5.13
	H36	4.11	H49	4.24
	H35	3.76	H36	3.99
	H49	3.74	H50	3.75
	H50	3.50	H35	3.72
	H47	3.29	H47	3.35
	H43	3.16	H43	3.23
	H51	2.95	H51	3.17
	H40	2.92	H40	3.00
	H45	2.62	H45	2.60
	H42	2.38	H42	2.42
	H46	1.86	H46	1.91
^{13}C	C31	202.11	C31	204.40
	C33	200.08	C33	202.44
	C9	192.78	C9	192.32
	C6	184.61	C6	185.82
	C37	181.60	C37	182.60
	C7	175.60	C7	176.42
	C12	156.77	C12	157.10
	C10	154.56	C10	155.33
	C20	153.25	C20	152.90
	C19	151.86	C23	151.62
	C23	150.70	C19	151.25
	C24	150.32	C24	150.91
	C21	144.10	C21	145.04

	C25	143.69	C25	144.36
	C11	143.25	C11	144.30
	C17	139.06	C16	140.62
	C16	139.05	C17	138.81
	C15	135.89	C15	136.22
	C18	132.68	C18	133.86
	C8	70.94	C8	70.81
	C39	47.13	C39	47.59
	C38	45.13	C38	45.52
	C48	39.50	C48	40.08
	C41	34.96	C41	35.19

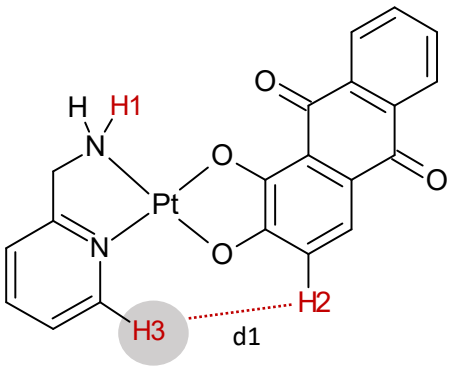
6b



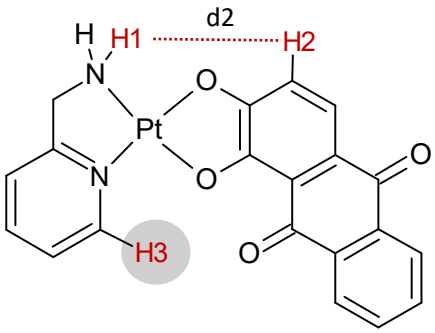
	Label	*δ (ppm)*	*Label*	*δ (ppm)*
^{1}H	H12	9.23	H12	9.62
	H23	9.02	H23	9.13
	H31	8.94	H31	9.01
	H15	8.41	H15	8.48
	H29	8.41	H29	8.48
	H27	8.40	H27	8.45
	H30	8.38	H30	8.44
	H14	8.10	H14	8.26
	H28	7.43	H28	7.47
	H45	4.77	H45	4.80
	H37	4.52	H37	4.59
	H36	3.76	H36	3.75
	H48	3.35	H48	3.39
	H44	3.09	H41	3.26
	H41	3.04	H44	3.13
	H43	2.60	H43	2.65
	H47	2.29	H47	2.19
	H46	2.01	H46	2.12
^{13}C	C32	202.06	C32	204.92
	C34	200.29	C34	202.33
	C6	191.95	C6	193.25
	C9	186.07	C9	185.13
	C7	179.53	C7	179.34
	C38	164.04	C38	165.35
	C10	156.56	C10	158.26
	C13	155.24	C13	155.40
	C21	153.31	C21	152.86
	C20	151.71	C24	151.69
	C24	150.78	C20	151.41
	C25	150.26	C25	151.07
	C22	144.13	C22	145.03
	C26	143.70	C26	144.50
	C11	142.69	C11	143.35
	C17	139.65	C17	140.45
	C18	138.65	C18	139.23

C16	136.19	C16	136.40
C19	132.70	C19	134.60
C8	73.40	C8	72.23
C40	44.13	C40	45.12
C39	42.26	C39	43.73
C42	32.55	C42	34.07

Table TS2. The shortest H-H distance (Å) between N^N and aliz ligands computed in DMSO for the depicted isomers *cis* and *trans* of complexes **3b**-**6b**, where H3 can be phenyl H (**3b**, **4b** and **6b**) or methyl H (**5b**).



cis isomer



trans isomer

	3b		**4b**		**5b**		**6b**	
	cis	*trans*	*cis*	*trans*	*cis*	*trans*	*cis*	*trans*
d1	4.613		4.322		3.849		4.373	
d2		5.304		5.335		5.051		5.497

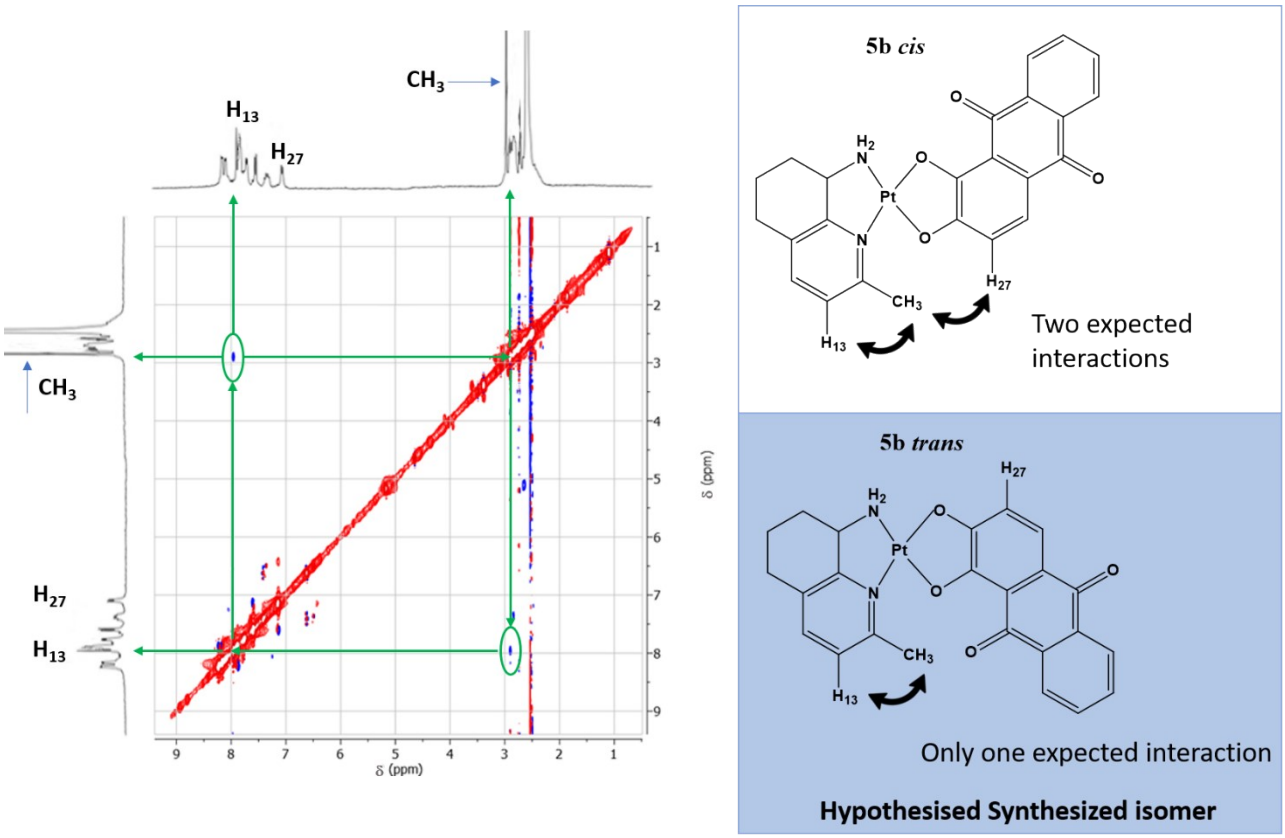


Figure S16. NOESY bidimensional experiment of complex **5b**. Note that proton numbers (H_{13} and H_{27}) are relative to the numbering used in Table S1.

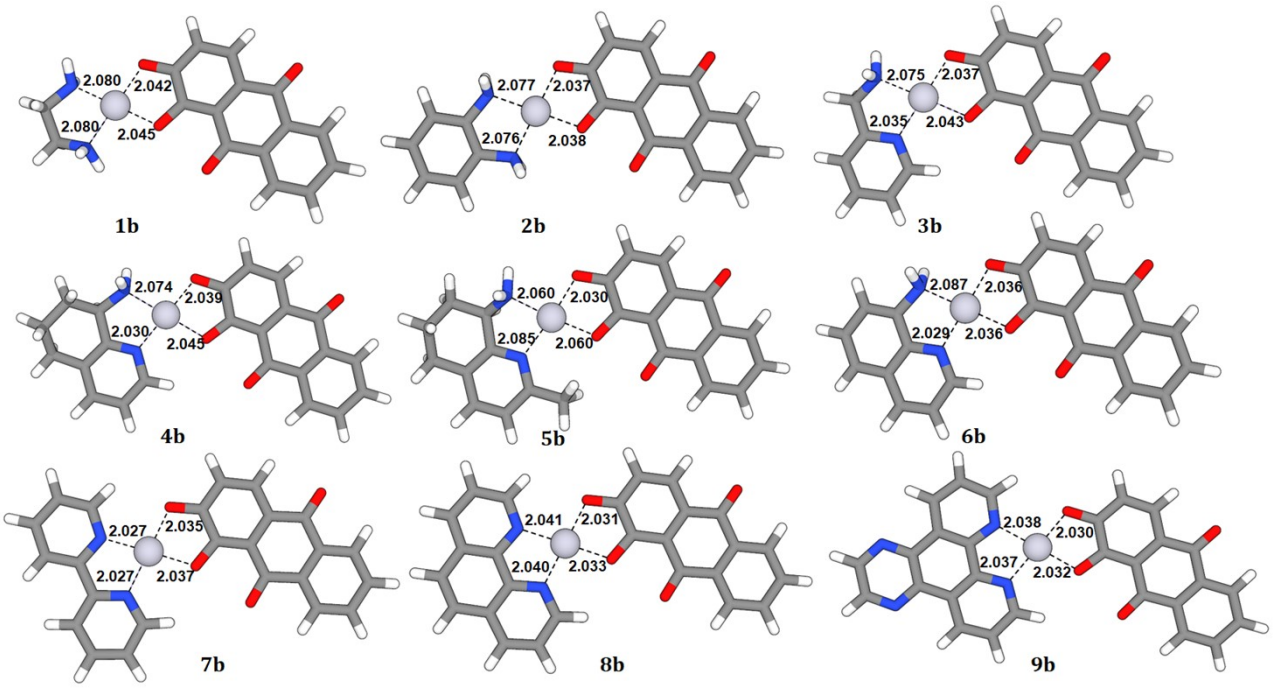


Figure S17. Optimized structure of complexes **1b**-**9b**. Bond distances in Å are reported.

Table TS3. Cartesian Coordinates of the optimized structures for the complexes.

1b

Atomic number	x	y	z
78	-0.910122	-1.251887	-0.743086
8	-0.871532	0.391788	-1.957562
8	1.095772	-0.879837	-0.665257
7	-2.952606	-1.628596	-0.843320
7	-0.955362	-2.908089	0.514404
6	1.416812	0.197610	-1.400079
6	-3.351603	-2.565316	0.254411
6	0.363250	0.886843	-2.095066
6	0.669019	2.030121	-2.873447
6	2.034519	2.465288	-2.945969
6	3.031867	1.768059	-2.263274
6	2.733161	0.644217	-1.495339
6	1.369699	4.401107	-4.436598
6	0.027755	3.980229	-4.373165
6	-0.955575	4.712817	-5.051121
1	-1.986406	4.381452	-4.997004
6	-0.612090	5.848336	-5.780983
6	0.722581	6.265040	-5.843413
6	1.707378	5.543154	-5.174269
1	4.055218	2.117931	-2.337650
1	3.513059	0.106252	-0.964298
1	-1.382135	6.409622	-6.301340
1	0.990741	7.150036	-6.412303
1	2.746139	5.852333	-5.212399
6	-0.375870	2.766622	-3.599290
8	-1.573316	2.431813	-3.599843
6	2.432741	3.645325	-3.726161
8	3.617065	4.018557	-3.798834
6	-2.267710	-3.616957	0.379900
1	-0.188965	-3.554603	0.324397
1	-0.838160	-2.594044	1.479792
1	-2.219796	-4.232600	-0.521366
1	-2.441313	-4.264752	1.242691
1	-3.433421	-1.980984	1.173842
1	-3.502787	-0.770811	-0.787683
1	-3.168296	-2.054437	-1.746896
1	-4.321162	-3.019459	0.035152

2b

Atomic number	x	y	z
78	-1.744085	-0.327380	-0.000052
8	0.143607	0.439021	0.000011
8	-0.718142	-2.088677	-0.000223
6	1.077023	-0.514911	-0.000065
6	0.605657	-1.876089	-0.000191
7	-2.761322	1.482573	0.000017
7	-3.670974	-1.104212	-0.000021
6	-4.211047	1.276493	0.000141
6	-4.672318	-0.034760	0.000110
6	-6.475996	2.078762	0.000389
6	-6.039095	-0.305524	0.000212
1	-7.181242	2.903488	0.000503
1	-4.730717	3.362279	0.000313
6	-6.940514	0.758982	0.000351
6	-5.106573	2.343861	0.000283
1	-8.006857	0.558052	0.000432
1	-6.383802	-1.334882	0.000183
6	1.510474	-2.934062	-0.000276
6	2.467659	-0.254127	-0.000031
6	2.879435	-2.675283	-0.000245
1	1.131517	-3.951419	-0.000369
6	3.374010	-1.369456	-0.000124
6	2.987112	1.116741	0.000102
1	3.580636	-3.501973	-0.000311
6	4.825673	-1.179327	-0.000086
6	4.467445	1.307236	0.000140
8	2.250393	2.125338	0.000226
6	5.350042	0.208240	0.000050
8	5.621187	-2.146601	-0.000128
6	4.989163	2.607681	0.000274
6	6.733975	0.428760	0.000095
6	6.366183	2.817175	0.000318
1	4.307405	3.450591	0.000345
1	7.403684	-0.423965	0.000025
6	7.241239	1.725373	0.000228
1	6.758445	3.829359	0.000424
1	8.314627	1.887223	0.000262
1	-2.494994	2.039136	-0.817016
1	-2.494857	2.039185	0.816971
1	-3.813852	-1.704228	0.817122
1	-3.813954	-1.704119	-0.817227

3b-cis

Atomic number	x	y	z
78	-1.977880	-0.560751	-0.103532
7	-3.884743	-1.376659	-0.159081
7	-3.079140	1.149859	-0.081954
8	-0.885424	-2.316613	-0.049703
8	0.041529	0.182562	-0.199740

3b-trans

Atomic number	x	y	z
78	-1.977880	-0.560751	-0.103532
7	-3.884743	-1.376659	-0.159081
7	-3.079140	1.149859	-0.081954
8	-0.110965	0.266790	-0.055351
8	-0.893108	-2.285186	-0.112787

1	-4.136312	-1.566376	-1.131197	1	-4.136312	-1.566376	-1.131197
6	-4.858667	-0.410101	0.429803	6	-4.858667	-0.410101	0.429803
1	-3.941903	-2.266236	0.337311	1	-3.941903	-2.266236	0.337311
6	-4.412170	0.993003	0.131233	6	-4.412170	0.993003	0.131233
6	-2.572495	2.379818	-0.316067	6	-2.572495	2.379818	-0.316067
1	-4.864464	-0.564930	1.512951	1	-4.864464	-0.564930	1.512951
1	-5.866775	-0.595164	0.052335	1	-5.866775	-0.595164	0.052335
6	0.442859	-2.164951	-0.068394	6	0.852133	-0.660621	-0.049102
6	0.936917	-0.818391	-0.147621	6	0.426513	-2.032256	-0.081657
6	-5.272016	2.085726	0.109665	6	-5.272016	2.085726	0.109665
6	-3.382315	3.505886	-0.336711	6	-3.382315	3.505886	-0.336711
1	-1.504131	2.431912	-0.486668	1	-1.504131	2.431912	-0.486668
6	1.358245	-3.243907	-0.014260	6	2.234922	-0.357907	-0.013513
6	2.307434	-0.569576	-0.170156	6	1.364234	-3.062503	-0.079621
6	-4.753215	3.358254	-0.121904	6	-4.753215	3.358254	-0.121904
1	-6.332329	1.929903	0.274939	1	-6.332329	1.929903	0.274939
1	-2.938412	4.476553	-0.524848	1	-2.938412	4.476553	-0.524848
6	0.896293	-4.636525	0.066328	6	2.713982	1.030817	0.021507
6	2.762655	-2.953566	-0.040120	6	3.174301	-1.441833	-0.011600
6	3.206758	-1.633131	-0.116838	6	2.724901	-2.762295	-0.044497
1	2.657347	0.456839	-0.229934	1	1.018628	-4.091799	-0.105050
1	-5.410518	4.221199	-0.139846	1	-5.410518	4.221199	-0.139846
6	1.926368	-5.717684	0.119352	6	4.189205	1.265606	0.058401
8	-0.304957	-4.955232	0.092091	8	1.953229	2.013921	0.022070
6	3.774810	-4.018210	0.011945	6	4.625246	-1.209314	0.024879
1	4.274025	-1.443472	-0.134979	1	3.457586	-3.561372	-0.041982
6	3.303037	-5.424225	0.093354	6	5.104643	0.196035	0.060189
6	1.508099	-7.052510	0.197012	6	4.667889	2.581852	0.091556
8	4.993304	-3.770064	-0.010243	8	5.442557	-2.146756	0.026603
6	4.237769	-6.466383	0.144726	6	6.480416	0.457680	0.095484
6	2.443788	-8.083048	0.247856	6	6.037369	2.833677	0.126414
1	0.445729	-7.268258	0.216760	1	3.954955	3.398729	0.089601
6	3.812131	-7.789941	0.221624	6	6.946391	1.769422	0.128464
1	5.294201	-6.222261	0.123439	1	7.171394	-0.378170	0.096620
1	2.109428	-9.114223	0.307812	1	6.398224	3.857317	0.152063
1	4.541688	-8.593006	0.261163	1	8.013900	1.965410	0.155710

4b-cis

Atomic number	x	y	z
78	-0.852266	-0.995129	-0.324163
8	1.098802	-0.458298	-0.041166
8	-0.801083	0.648325	-1.538380
7	-2.794955	-1.514071	-0.589072
7	-0.909943	-2.687683	0.897567
6	0.401105	1.211108	-1.546123
6	-3.264358	-2.484925	0.221380
6	-2.320279	-3.101968	1.213966
6	1.436546	0.616529	-0.733743
6	-4.585882	-2.923530	0.175628
6	-4.939279	-1.349649	-1.611986
1	-3.182312	-0.174537	-2.112561
6	-5.431191	-2.345304	-0.769009

4b-trans

Atomic number	x	y	z
78	-0.890696	-1.167513	-0.623704
8	-0.878050	0.421409	-1.910598
8	1.099272	-0.733326	-0.536915
7	-2.872643	-1.602187	-0.687192
7	-0.904477	-2.789481	0.670423
6	1.407158	0.309864	-1.325824
6	-3.298068	-2.532216	0.198727
6	-2.290142	-3.124915	1.140640
6	0.345132	0.939205	-2.061080
6	-4.639186	-2.909297	0.297088
6	-5.103713	-1.366964	-1.498606
1	-3.360033	-0.293859	-2.219742
6	-5.550948	-2.315498	-0.577020

1	-5.572090	-0.880241	-2.353552	1	-5.787606	-0.888611	-2.190344
1	-6.464141	-2.665476	-0.841610	1	-6.600360	-2.591286	-0.535765
6	2.728152	1.195182	-0.716403	6	0.631988	2.049493	-2.891703
6	2.971038	2.361317	-1.519446	6	1.989290	2.504975	-2.983564
6	1.946102	2.904646	-2.292463	6	2.996583	1.863810	-2.261719
6	0.672825	2.342767	-2.310220	6	2.715048	0.776444	-1.436508
6	5.372797	2.440169	-0.729571	6	1.294564	4.335183	-4.590034
6	5.144132	1.302552	0.061583	6	-0.041153	3.899043	-4.499923
6	6.190154	0.782508	0.833250	6	-1.034212	4.569662	-5.225987
1	6.002077	-0.094774	1.438880	1	-2.060314	4.228131	-5.150045
6	7.444335	1.382056	0.820351	6	-0.706229	5.657759	-6.031373
6	7.670217	2.514960	0.032076	6	0.622151	6.089305	-6.120737
6	6.638663	3.038819	-0.737547	6	1.616271	5.430037	-5.402488
1	2.159087	3.783750	-2.887152	1	4.013751	2.227823	-2.351308
1	-0.121292	2.769864	-2.912282	1	3.501905	0.282026	-0.874357
1	8.246729	0.970559	1.421928	1	-1.483528	6.170499	-6.589647
1	8.647507	2.983699	0.021225	1	0.878210	6.937360	-6.748399
1	6.794078	3.915092	-1.354142	1	2.650127	5.752334	-5.459688
6	3.805216	0.624873	0.105375	6	-0.426587	2.733906	-3.646929
8	3.668064	-0.368311	0.822493	8	-1.621214	2.392200	-3.607603
6	4.282809	3.019414	-1.562698	6	2.367791	3.646748	-3.828175
8	4.501928	4.019609	-2.256752	8	3.544211	4.040905	-3.914649
1	-0.436993	-3.442883	0.401215	1	-0.511329	-3.591977	0.173924
1	-0.390224	-2.547728	1.761317	1	-0.300850	-2.628891	1.477407
6	-3.618239	-0.949030	-1.496147	6	-3.759088	-1.026977	-1.529830
6	-4.994071	-3.956207	1.190529	6	-4.980895	-3.930755	1.348992
6	-2.479977	-4.632761	1.217743	6	-2.485032	-4.646841	1.330922
1	-1.879955	-5.046240	2.030372	1	-1.992786	-4.933863	2.264054
6	-3.958274	-5.097951	1.326239	6	-3.972614	-5.097821	1.325791
1	-4.123723	-5.599152	2.281247	1	-4.165283	-5.752006	2.180074
1	-5.095260	-3.449168	2.157778	1	-4.956829	-3.445224	2.334343
1	-2.554502	-2.697236	2.203001	1	-2.418299	-2.623149	2.106558
1	-2.052460	-5.003189	0.281134	1	-1.956220	-5.157464	0.518396
1	-4.147460	-5.836741	0.545254	1	-4.160790	-5.689015	0.424439
1	-5.977402	-4.362593	0.948585	1	-5.998735	-4.301182	1.200603

5b-cis				**5b-trans**			
Atomic number	x	y	z	Atomic number	x	y	z
78	-0.932845	-1.068768	-0.904391	78	-1.069411	-1.256320	-0.985069
8	1.079153	-0.759899	-0.829723	8	-0.943402	0.482438	-2.083992
8	-0.804558	0.610603	-2.091133	8	0.949152	-1.033733	-0.994577
7	-0.923203	-2.707943	0.363490	7	-1.070554	-2.944807	0.195156
7	-2.962210	-1.536913	-0.885620	7	-3.116102	-1.629553	-0.859449
6	1.478162	0.291617	-1.524891	6	0.315484	0.896005	-2.231580
6	-3.301526	-2.436444	0.083933	6	-3.430815	-2.515579	0.134848
6	-2.223812	-2.717773	1.105715	6	-2.291181	-2.876414	1.057943
6	0.444032	1.034088	-2.202584	6	1.336856	0.073177	-1.647755
6	-4.550063	-3.041983	0.143889	6	-4.707945	-3.048232	0.293199
6	-5.179919	-1.679301	-1.734523	6	-5.394870	-1.665286	-1.555280
6	-5.506297	-2.634762	-0.788763	6	-5.706429	-2.592326	-0.573386
1	-5.910766	-1.352227	-2.462475	1	-6.154727	-1.306383	-2.240054
1	-6.495359	-3.078887	-0.777581	1	-6.716728	-2.981302	-0.486015
6	2.825679	0.706200	-1.631784	6	0.684454	2.077434	-2.923422
6	3.125568	1.872652	-2.414693	6	2.077660	2.407636	-3.020906
6	2.098780	2.570705	-3.049959	6	3.040633	1.579181	-2.444234
6	0.772012	2.163110	-2.951335	6	2.680795	0.419069	-1.760193

6	5.589564	1.609084	-1.909836	6	1.521284	4.502752	-4.330330
6	5.305882	0.466646	-1.143434	6	0.152349	4.187719	-4.237171
6	6.356118	-0.226325	-0.529683	6	-0.791767	5.043178	-4.820084
1	6.124303	-1.105132	0.058399	1	-1.843656	4.792072	-4.742804
6	7.669172	0.206678	-0.674692	6	-0.383067	6.195723	-5.486908
6	7.950060	1.344556	-1.437670	6	0.978317	6.507317	-5.579032
6	6.914469	2.040088	-2.050022	6	1.924438	5.663729	-5.002904
1	2.355069	3.446839	-3.631951	1	4.085176	1.854689	-2.535393
1	-0.021903	2.708026	-3.449588	1	3.432900	-0.222606	-1.310541
1	8.474641	-0.338409	-0.195999	1	-1.122789	6.852013	-5.935132
1	8.973268	1.683703	-1.551558	1	1.297343	7.405450	-6.098962
1	7.112788	2.922992	-2.644476	1	2.982912	5.891357	-5.065356
6	3.903121	-0.035195	-0.962202	6	-0.322039	2.959034	-3.530047
8	3.715666	-1.037178	-0.269154	8	-1.544130	2.735325	-3.482714
6	4.496465	2.369067	-2.578481	6	2.542928	3.613769	-3.721072
8	4.763770	3.377690	-3.243459	8	3.750552	3.897985	-3.810916
1	-0.808371	-3.572784	-0.166245	1	-1.088777	-3.799337	-0.367726
1	-0.144236	-2.658642	1.018406	1	-0.235269	-2.993579	0.781191
6	-3.889082	-1.148476	-1.793921	6	-4.083726	-1.202356	-1.711212
6	-4.805828	-4.145358	1.141605	6	-4.949100	-4.133142	1.315705
6	-2.449662	-3.974772	1.976280	6	-2.515723	-4.131506	1.932705
1	-2.763151	-3.644968	2.970261	1	-2.702793	-3.795544	2.957760
6	-3.512422	-4.920999	1.413082	6	-3.692704	-4.997425	1.474737
1	-3.695328	-5.729009	2.124775	1	-3.867573	-5.790712	2.207742
1	-5.185212	-3.723044	2.080093	1	-5.211900	-3.687542	2.284996
1	-2.174301	-1.840289	1.755694	1	-2.120305	-2.015921	1.712700
1	-1.495531	-4.491671	2.107720	1	-1.588076	-4.713439	1.957894
1	-3.163834	-5.380880	0.481966	1	-3.462718	-5.482668	0.517867
1	-5.586110	-4.804132	0.753833	1	-5.807712	-4.733910	1.001069
6	-3.511276	-0.162696	-2.853767	6	-3.746626	-0.247622	-2.813848
1	-3.184893	0.777500	-2.407960	1	-3.471596	0.731593	-2.413055
1	-2.668138	-0.530322	-3.441753	1	-2.900557	-0.608415	-3.403731
1	-4.357244	0.023696	-3.514387	1	-4.609794	-0.123303	-3.470243

6b-cis

Atomic number	x	y	z
78	-1.226543	-1.221490	-0.836721
8	-1.076310	0.427237	-2.029531
8	0.777548	-0.908063	-0.653501
7	-3.282929	-1.527586	-1.031735
7	-1.395428	-2.857696	0.351024
6	0.175362	0.887179	-2.106081
6	-2.680197	-3.346988	0.465527
6	-3.702902	-2.683006	-0.239187
6	1.170408	0.161685	-1.359372
6	-2.977219	-4.481451	1.265657
6	-0.626600	-4.594601	1.812113
1	0.584469	-3.039442	0.879062
6	-1.899900	-5.103171	1.946485
1	0.219361	-5.045050	2.317540
1	-2.093235	-5.973493	2.565651
6	0.555718	2.019734	-2.864297
6	1.937742	2.414343	-2.858668
6	2.873333	1.685176	-2.122090
6	2.501451	0.568119	-1.377554

6b-trans

Atomic number	x	y	z
78	-0.893505	-1.249289	-0.737509
8	-0.865276	0.404972	-1.924909
8	1.111304	-0.896508	-0.690870
7	-0.926153	-2.941790	0.481746
7	-2.891372	-1.603578	-0.777674
6	0.371572	0.889035	-2.088447
6	-3.287803	-2.699963	-0.041507
6	-2.293962	-3.433636	0.635161
6	1.431303	0.185781	-1.422531
6	-4.651051	-3.089519	0.041726
6	-5.175539	-1.216106	-1.390926
1	-3.443846	-0.037113	-1.992438
6	-5.600054	-2.306044	-0.663548
1	-5.873320	-0.595875	-1.941096
1	-6.650691	-2.575590	-0.620780
6	0.669767	2.032660	-2.867766
6	2.036713	2.455660	-2.965838
6	3.041931	1.746741	-2.307022
6	2.749365	0.620404	-1.539927

6	1.415213	4.357714	-4.390438	6	1.357659	4.401079	-4.438999
6	0.058847	3.974962	-4.404656	6	0.013832	3.990623	-4.350696
6	-0.859912	4.729348	-5.146373	6	-0.976539	4.731326	-5.009153
1	-1.902535	4.432772	-5.154699	1	-2.008704	4.407894	-4.935939
6	-0.441331	5.847347	-5.863948	6	-0.638109	5.864901	-5.744412
6	0.905668	6.225677	-5.849411	6	0.698271	6.271441	-5.831463
6	1.827546	5.483390	-5.116102	6	1.690049	5.541394	-5.181651
1	3.910301	2.000496	-2.133340	1	4.066478	2.088333	-2.400394
1	3.232864	0.004346	-0.806773	1	3.534904	0.071906	-1.028460
1	-1.162833	6.424179	-6.434169	1	-1.413448	6.432495	-6.249816
1	1.233261	7.096713	-6.408300	1	0.962459	7.154940	-6.404495
1	2.873481	5.768506	-5.097973	1	2.730167	5.842844	-5.239357
6	-0.422473	2.782132	-3.647173	6	-0.384231	2.779793	-3.570282
8	-1.632316	2.479214	-3.709631	8	-1.583548	2.454109	-3.545514
6	2.408562	3.578403	-3.612397	6	2.428468	3.635824	-3.750639
8	3.611887	3.924620	-3.612715	8	3.613773	3.999561	-3.844713
1	-3.798195	-0.695997	-0.729874	1	-0.333985	-3.674721	0.082190
1	-3.530057	-1.673098	-2.014658	1	-0.528333	-2.723916	1.399195
6	-0.405406	-3.463361	1.002987	6	-3.805959	-0.888881	-1.428467
6	-4.325568	-4.918835	1.333721	6	-4.976341	-4.230663	0.820558
6	-5.003115	-3.122084	-0.160544	6	-2.630137	-4.537067	1.384613
1	-5.785315	-2.603832	-0.706193	1	-1.859165	-5.098317	1.903685
6	-5.310974	-4.252113	0.636418	6	-3.986853	-4.934383	1.473829
1	-6.340152	-4.590119	0.692013	1	-4.240409	-5.806156	2.067475
1	-4.563187	-5.784925	1.943057	1	-6.015429	-4.536189	0.890557

7b

Atomic number	x	y	z
78	-1.521037	-0.268502	-0.002590
8	0.401782	0.403815	-0.010286
8	-0.573824	-2.069781	0.003373
7	-2.483821	1.514976	-0.006959
7	-3.448292	-0.897029	0.006342
6	0.761991	-1.925694	0.000689
6	-3.847672	1.452172	-0.000015
6	1.294510	-0.593520	-0.003826
6	-4.610237	2.618934	0.002716
6	-2.574758	3.900869	-0.012295
1	-0.778553	2.683752	-0.018336
6	-3.968328	3.854887	-0.003218
1	-2.037203	4.841804	-0.016956
1	-4.551639	4.769222	-0.000553
6	2.696625	-0.397958	-0.001988
6	3.546255	-1.553028	-0.003995
6	2.993762	-2.834578	-0.003257
6	1.613692	-3.027807	0.000466
6	5.604150	-0.075356	-0.000555
6	4.777336	1.064034	0.006053
6	5.360788	2.337778	0.012749
1	4.716194	3.209471	0.018017
6	6.746498	2.479014	0.012547
6	7.567100	1.345338	0.005936
6	6.996877	0.074996	-0.000423
1	3.661409	-3.688585	-0.005050
1	1.187682	-4.026780	0.002516
1	7.188631	3.470599	0.017458

8b

Atomic number	x	y	z
78	-0.898044	-1.360968	-0.876509
8	-0.872272	0.353199	-1.970027
8	1.108098	-1.044281	-0.865796
7	-0.957475	-3.082286	0.218011
7	-2.911048	-1.692541	-0.880968
6	0.368994	0.826783	-2.142905
6	-3.275752	-2.822985	-0.202425
6	1.431151	0.069003	-1.547226
6	-4.613788	-3.245709	-0.080706
6	-5.216232	-1.302287	-1.379991
1	-3.529205	-0.061773	-1.984721
6	-5.599754	-2.442900	-0.697323
1	-5.947559	-0.665341	-1.863674
1	-6.645005	-2.727267	-0.630201
6	0.668828	2.005707	-2.867018
6	2.041387	2.402122	-2.986764
6	3.049664	1.639848	-2.395333
6	2.754822	0.481885	-1.678467
6	1.368400	4.424549	-4.356686
6	0.017736	4.045232	-4.239779
6	-0.972749	4.831788	-4.842346
1	-2.010256	4.532081	-4.746735
6	-0.627310	5.979352	-5.552244
6	0.715870	6.355126	-5.667551
6	1.707679	5.580357	-5.071691
1	4.078219	1.964785	-2.502773
1	3.541934	-0.108651	-1.218979
1	-1.402430	6.581689	-6.016058

1	8.647239	1.455061	0.005866
1	7.619021	-0.813228	-0.005290
6	3.287233	0.949322	0.005920
8	2.609627	1.991003	0.014957
6	5.012621	-1.437537	-0.007335
8	5.750524	-2.438031	-0.015744
6	-1.861368	2.708985	-0.013154
6	-4.392760	0.088882	0.003971
6	-5.749611	-0.230658	0.003653
6	-6.137054	-1.568344	0.008097
6	-3.821243	-2.190822	0.011366
6	-5.159496	-2.562593	0.012787
1	-3.019319	-2.918965	0.013814
1	-5.418942	-3.614712	0.016922
1	-7.190007	-1.828220	0.007787
1	-6.493498	0.556457	-0.000753
1	-5.691674	2.561734	0.011118

1	0.985406	7.249602	-6.220713
1	2.752856	5.858293	-5.151658
6	-0.388359	2.820101	-3.486449
8	-1.596601	2.539936	-3.411430
6	2.438600	3.609239	-3.728026
8	3.628771	3.951212	-3.836510
6	-3.859280	-0.948591	-1.456797
6	-2.223317	-3.571929	0.389132
6	-2.498243	-4.751549	1.108081
6	-1.395153	-5.435660	1.666451
6	0.070557	-3.744582	0.755351
6	-0.120794	-4.927844	1.487136
1	1.056847	-3.324320	0.598303
1	0.746141	-5.427663	1.903126
1	-1.557081	-6.349550	2.229073
6	-4.879773	-4.451367	0.655017
6	-3.867738	-5.171772	1.223396
1	-4.080363	-6.080690	1.776949
1	-5.910411	-4.777868	0.749095

9b

Atomic number	x	y	z
78	1.396880	1.983418	-1.464109
8	1.436986	3.692045	-2.563085
8	3.403709	2.287510	-1.447961
7	-0.615253	1.662361	-1.471716
7	1.318041	0.269910	-0.363373
6	3.736798	3.396729	-2.131861
6	-0.999548	0.543681	-0.791007
6	2.681565	4.158929	-2.732733
6	-2.339706	0.148749	-0.681850
6	-2.905605	2.087462	-1.995181
1	-1.196673	3.297430	-2.591833
6	-3.309507	0.954313	-1.306481
1	-3.626704	2.729166	-2.487627
1	-4.356378	0.683219	-1.244692
6	2.990094	5.334589	-3.458018
6	4.365164	5.722227	-3.574820
6	5.367280	4.955097	-2.979105
6	5.063443	3.800695	-2.260168
6	3.707559	7.746349	-4.950118
6	2.354262	7.375812	-4.835256
6	1.369924	8.167347	-5.441289
1	0.330382	7.874264	-5.347088
6	1.724053	9.311301	-6.152757
6	3.069810	9.678320	-6.266133
6	4.055561	8.898520	-5.666745
1	6.398063	5.273551	-3.084636
1	5.845578	3.206507	-1.796935
1	0.953708	9.917635	-6.619304
1	3.346079	10.569948	-6.820558
1	5.102646	9.169665	-5.745168
6	1.939056	6.154691	-4.080653
8	0.729123	5.882110	-4.006651
6	4.771380	6.925645	-4.317591
8	5.963810	7.259851	-4.423971

6	-1.547961	2.419863	-2.062480
6	0.055151	-0.216377	-0.187417
6	-0.209698	-1.386799	0.536341
6	0.885937	-2.070117	1.094953
6	2.351801	-0.389056	0.174978
6	2.163270	-1.564370	0.910640
1	3.335601	0.033897	0.010638
1	3.028741	-2.065119	1.328291
1	0.721955	-2.979201	1.660668
6	-2.640253	-1.065967	0.067780
6	-1.597314	-1.818165	0.663270
6	-3.131532	-3.308484	1.455169
6	-4.166159	-2.562179	0.864706
1	-3.357214	-4.213565	2.012013
1	-5.198909	-2.884987	0.961119
7	-1.859367	-2.945117	1.359245
7	-3.929291	-1.452562	0.177453

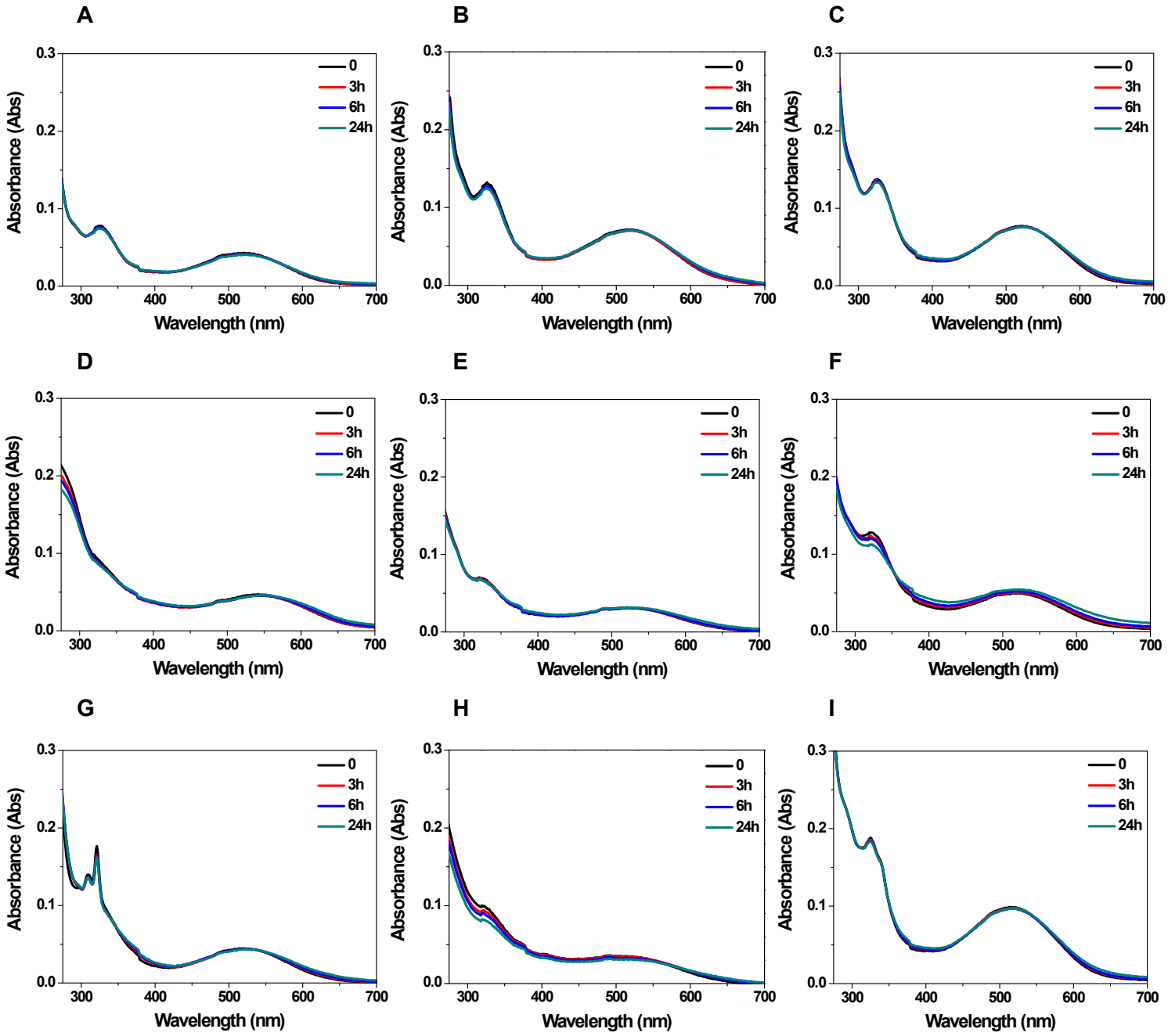


Figure S18. Absorption spectra over time (t = 0, 3, 6, and 24 h) of Pt(II) complexes [(N^N)Pt(aliz)] (A) **1b**, (B) **2b**, (C) **3b**, (D) **4b**, (E) **5b**, (F) **6b**, (G) **7b**, (H) **8b** and of (I) **9b** in DMSO/buffer solution (DMSO 0.5% v/v) at room temperature, $1 \cdot 10^{-5}$M.

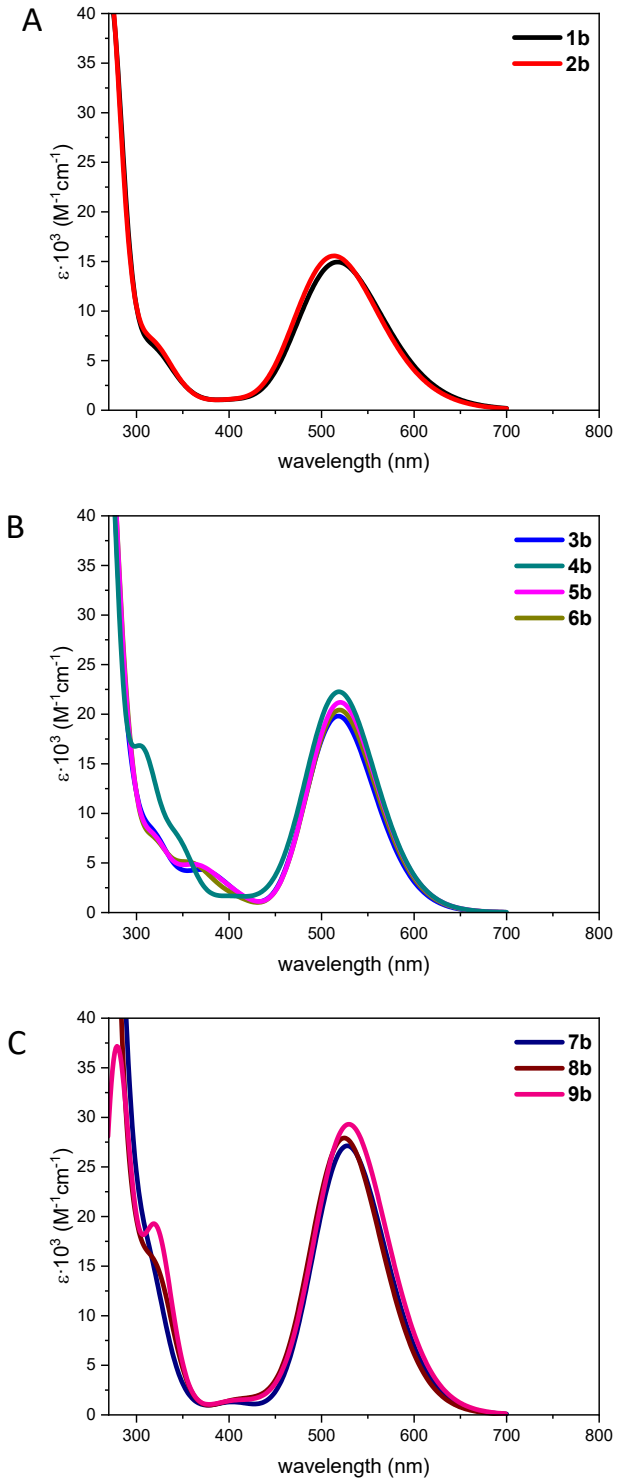


Figure S19. TDDFT simulated absorption spectra of Pt(II) complexes **1b**-**2b** (A), **3b**-**6b** (B), **7b**-**9b** (C) in aqueous environment.

Table TS4. TDDFT calculated electronic excitation energies (eV), absorption wavelength (nm), oscillator strength (*f*) and main configuration in water.

	Band	energy	wavelength	Main configuration	*f*	***Theoretical Assignment***
1b	I	2.40	517	H→L (99%)	0.277	$ML_{aliz}CT$
	II	3.91	318	H-4→L (80%)	0.072	$IL_{aliz}CT$
2b	I	2.42	513	H→L (99%)	0.288	$ML_{aliz}CT$
	II	3.90	318	H-4→L (70%)	0.075	$IL_{aliz}CT$
3b	I	2.39	518	H→L (99%)	0.294	$ML_{aliz}CT$
	II	3.90	318	H-5→L (88%)	0.070	$IL_{aliz}CT$
4b	I	2.39	519	H→L (99%)	0.303	$ML_{aliz}CT$
	II	3.90	318	H-5→L (82%)		$IL_{aliz}CT$
5b	I	2.38	520	H→L (99%)	0.314	$ML_{aliz}CT$
	II	3.91	318	H-6→L (87%)	0.075	$IL_{aliz}CT$
6b	I	2.39	520	H→L (99%)	0.325	$ML_{aliz}CT$
	II	3.89	319	H-5→L (65%)	0.064	$IL_{aliz}CT$
7b	I	2.34	529	H→L (93%)	0.396	MLCT
	II	3.89	319	H-5→L (78%)	0.076	$IL_{aliz}CT$
8b	I	2.34	531	H→L (92%)	0.422	MLCT
	II	3.83	324	H-5→L (78%)	0.101	$IL_{aliz}CT$
9b	I	2.36	525	H→L (94%)	0.410	MLCT
	II	3.88	319	H-4→L (59%)	0.102	MLCT/LLCT

[a]Only selected excited states were considered.

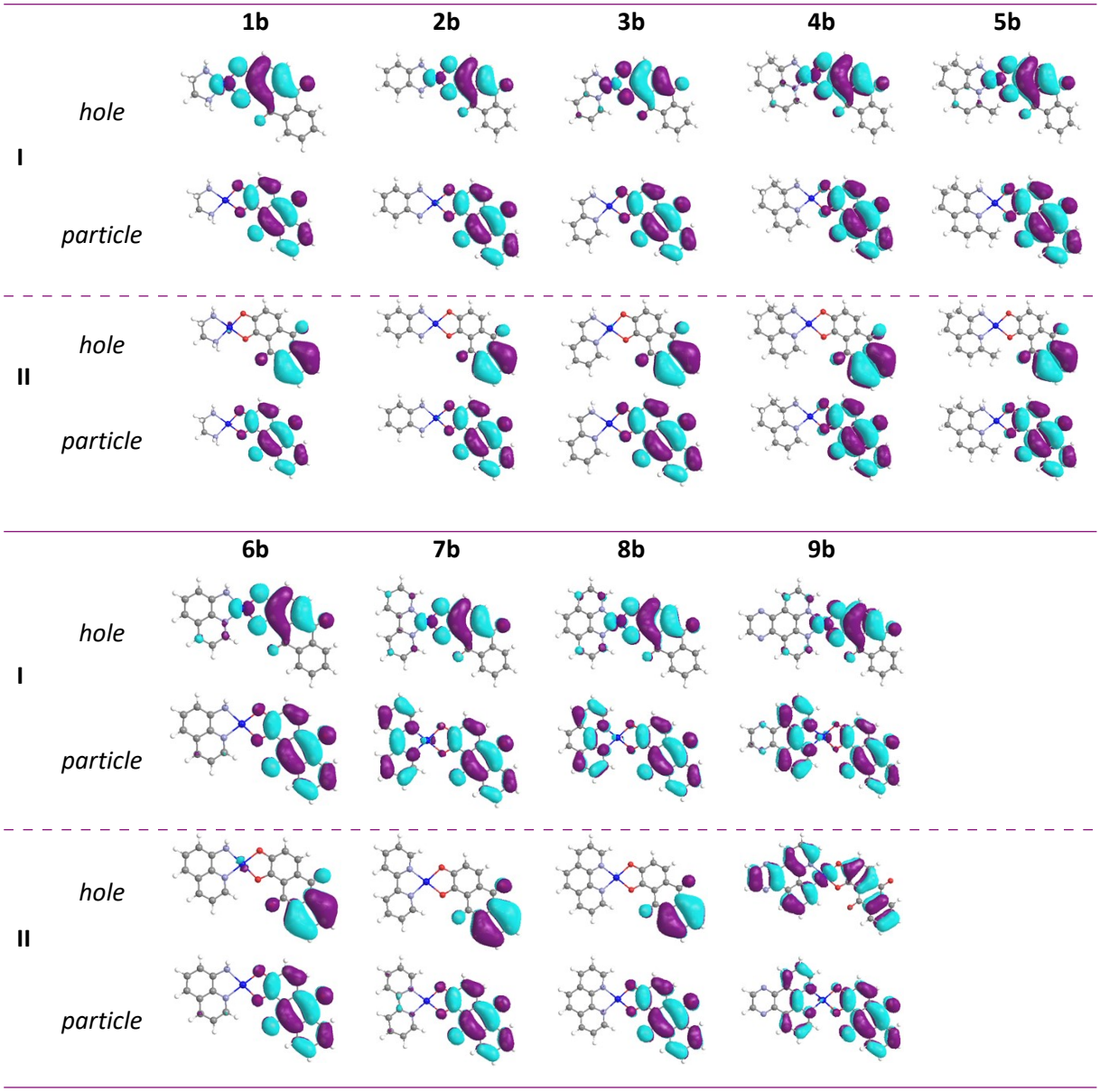


Figure S20. Natural Transition Orbitals (NTOs) for selected electronic transitions.

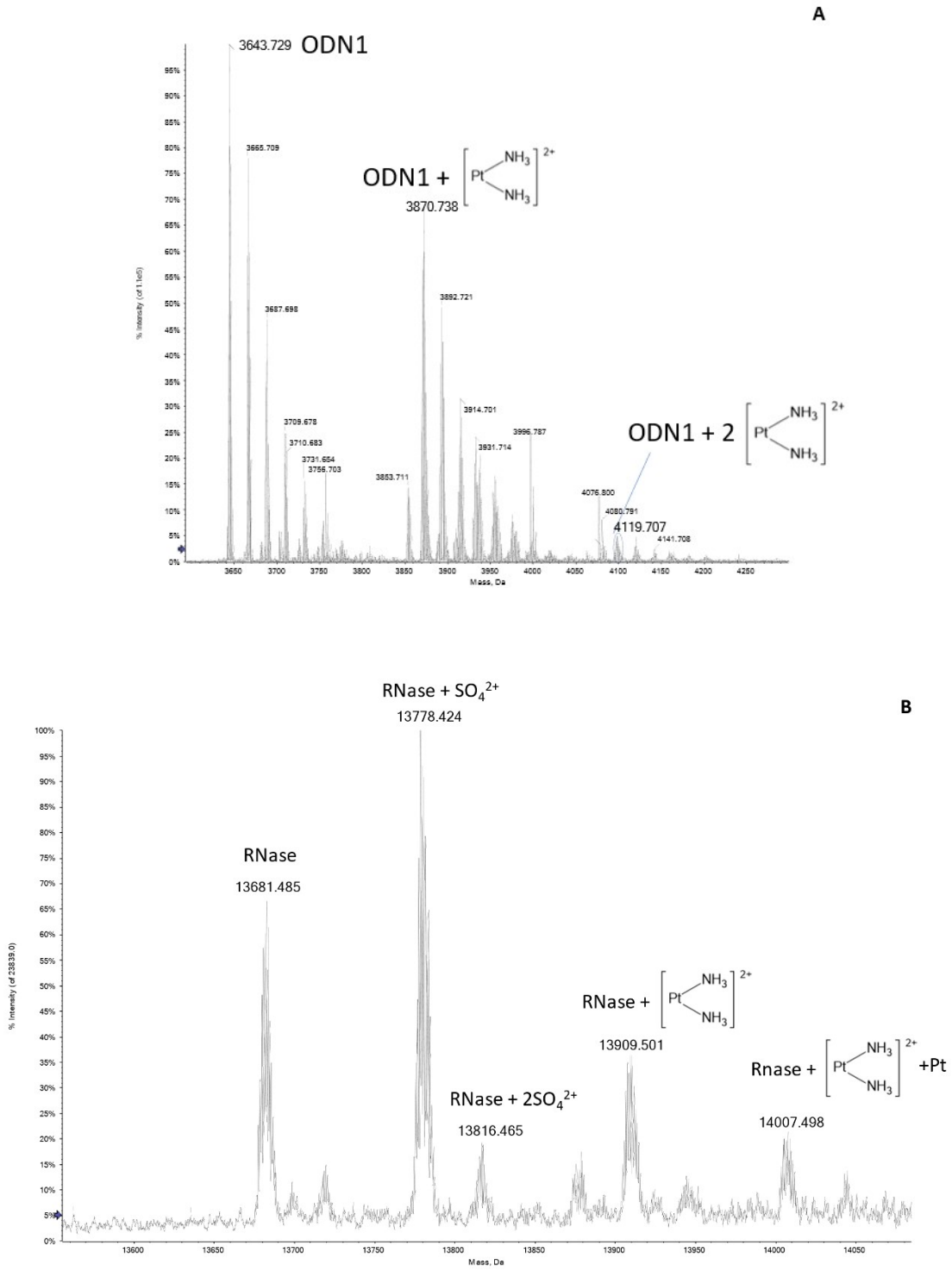


Figure S21. (A) Deconvoluted ESI-Q-TOF spectra of ODN with cisplatin; **(B)** Deconvoluted ESI-Q-TOF spectra of RNase with cisplatin in a 1:1 molecule to platinum ratio. All spectra were recorded at 24 h.

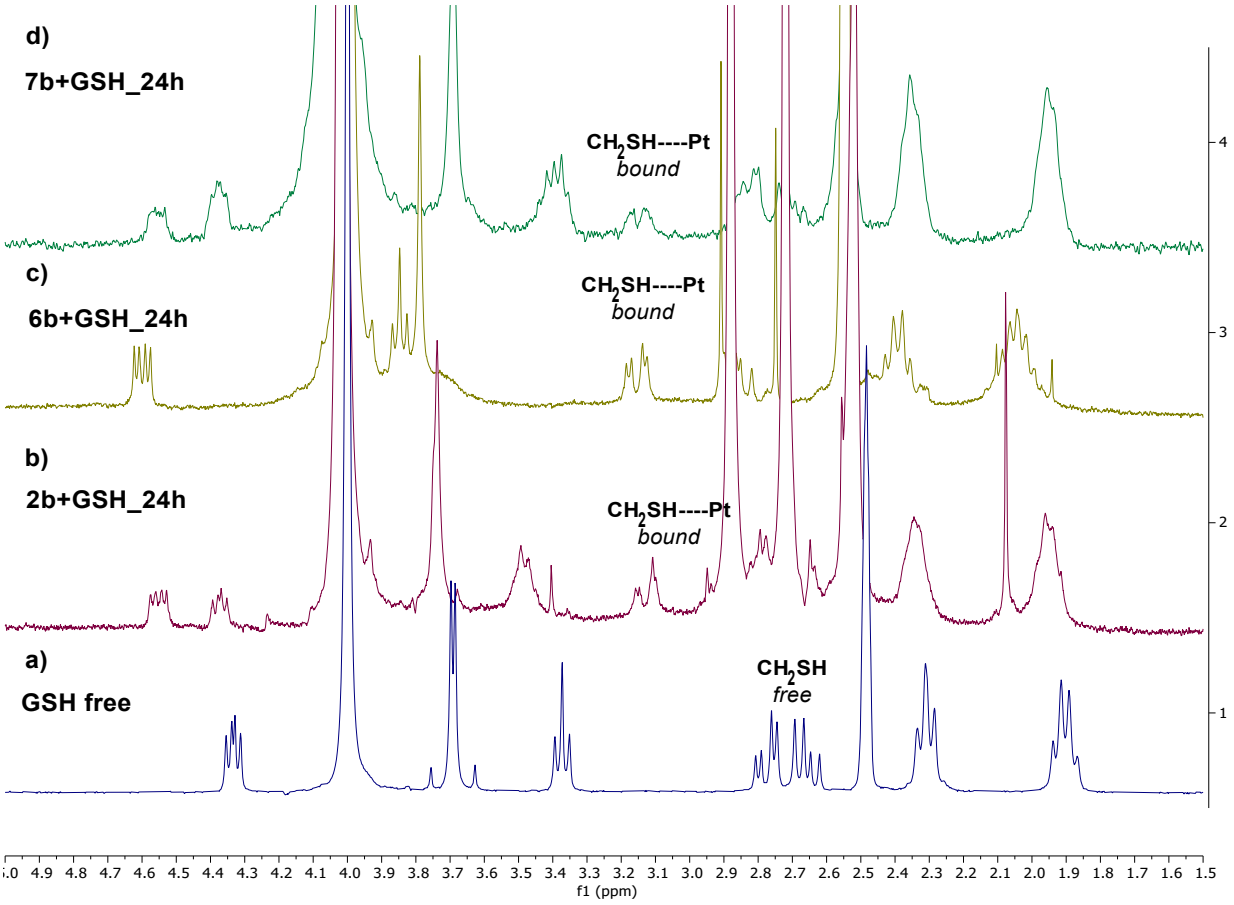


Figure S22. Binding study of GSH with compounds **2b**, **6b** and **7b** in 20 % physiological D_2O solution-DMSO-*d*6: stack plot of ^{1}H-NMR for aliphatic region.

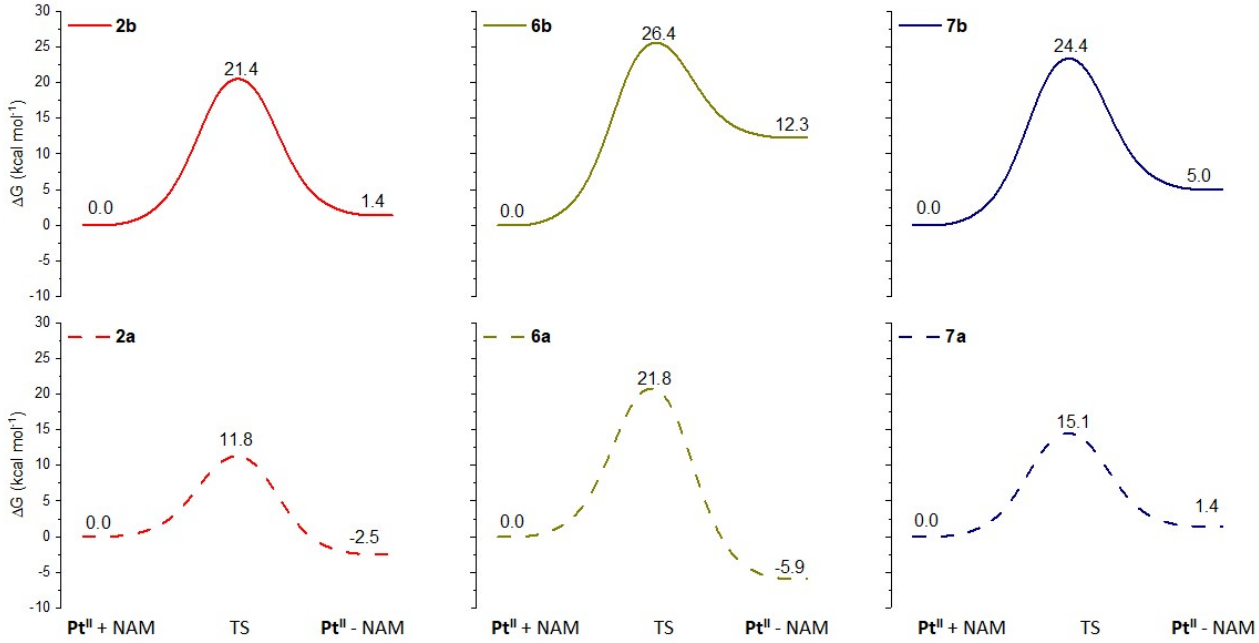


Figure S23. Free energy profiles for NAM attack to **Pt^{II}** complexes **2b**, **6b**, **7b**, **2a**, **6a** and **7a**.