Electronic Supplementary Information

Dyades of 5,15-diphenylporphyrin with pyrene

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NMR spectra

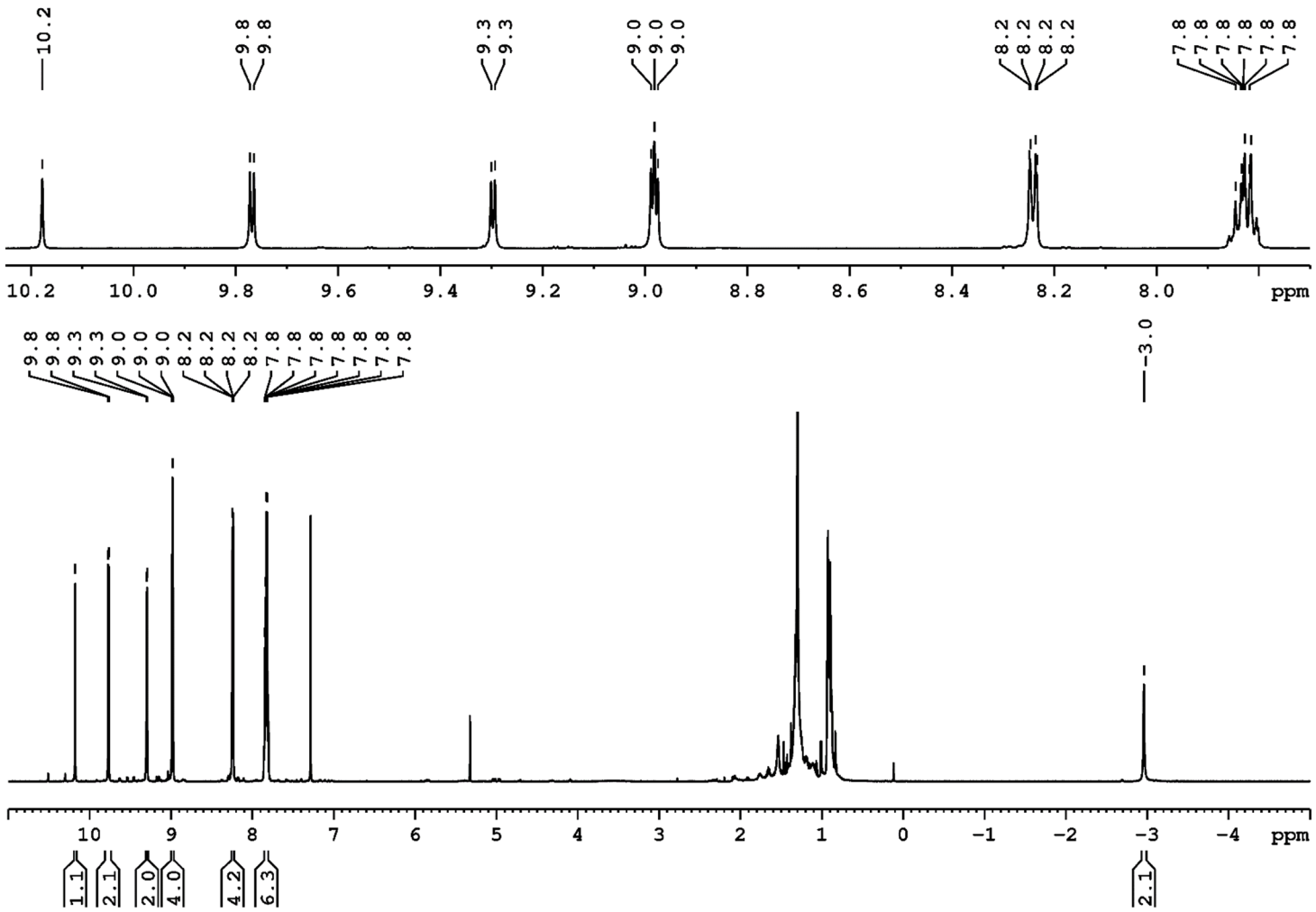

Figure S1. ^{1}H NMR spectrum of *5-bromo-10,20-diphenylporphyrin (**2**)* in $CDCl_3$.

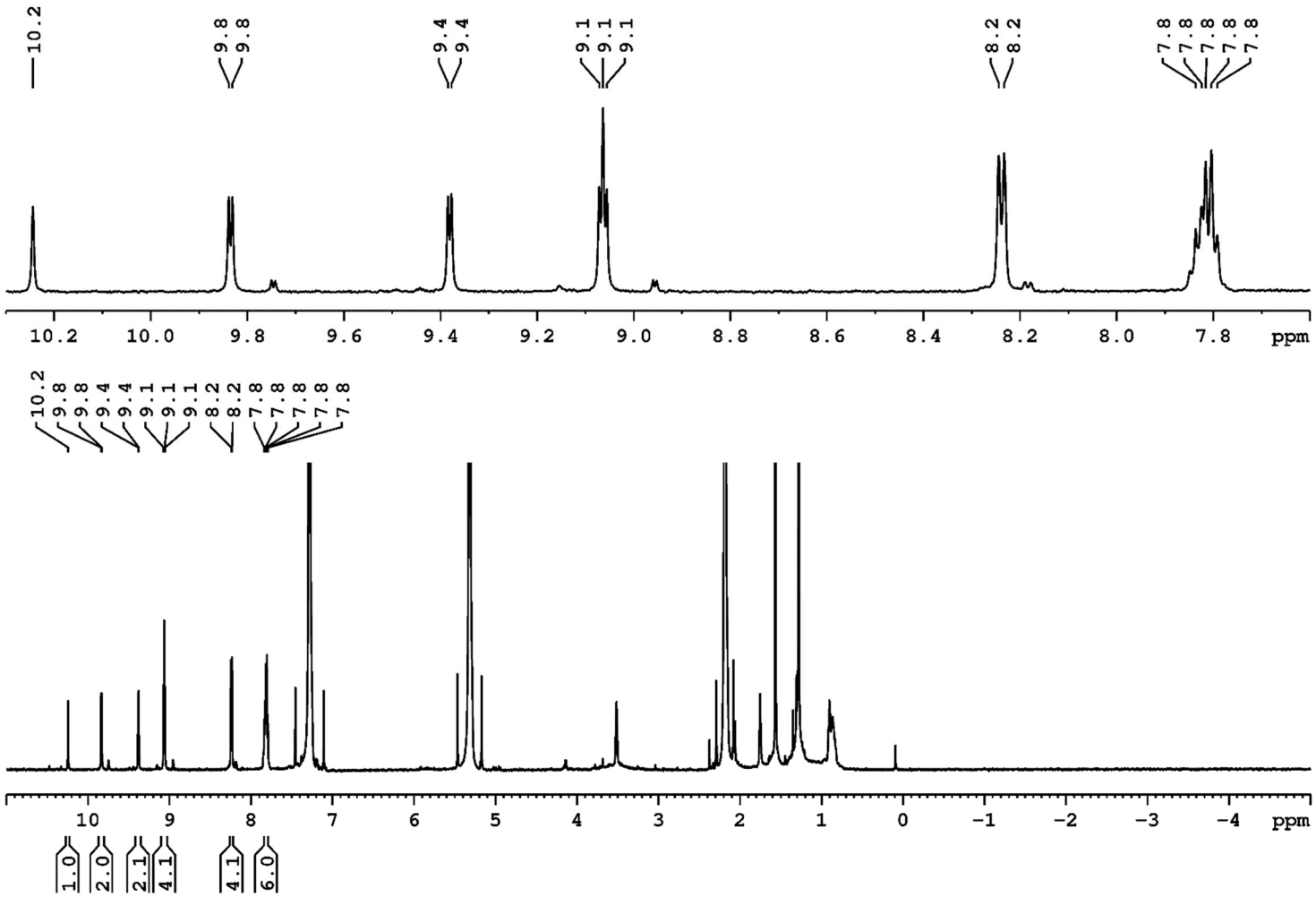

Figure S2. ^{1}H NMR spectrum of *Zn(II) 5-bromo-10,20-diphenylporphyrin (4)* in $CDCl_3$.

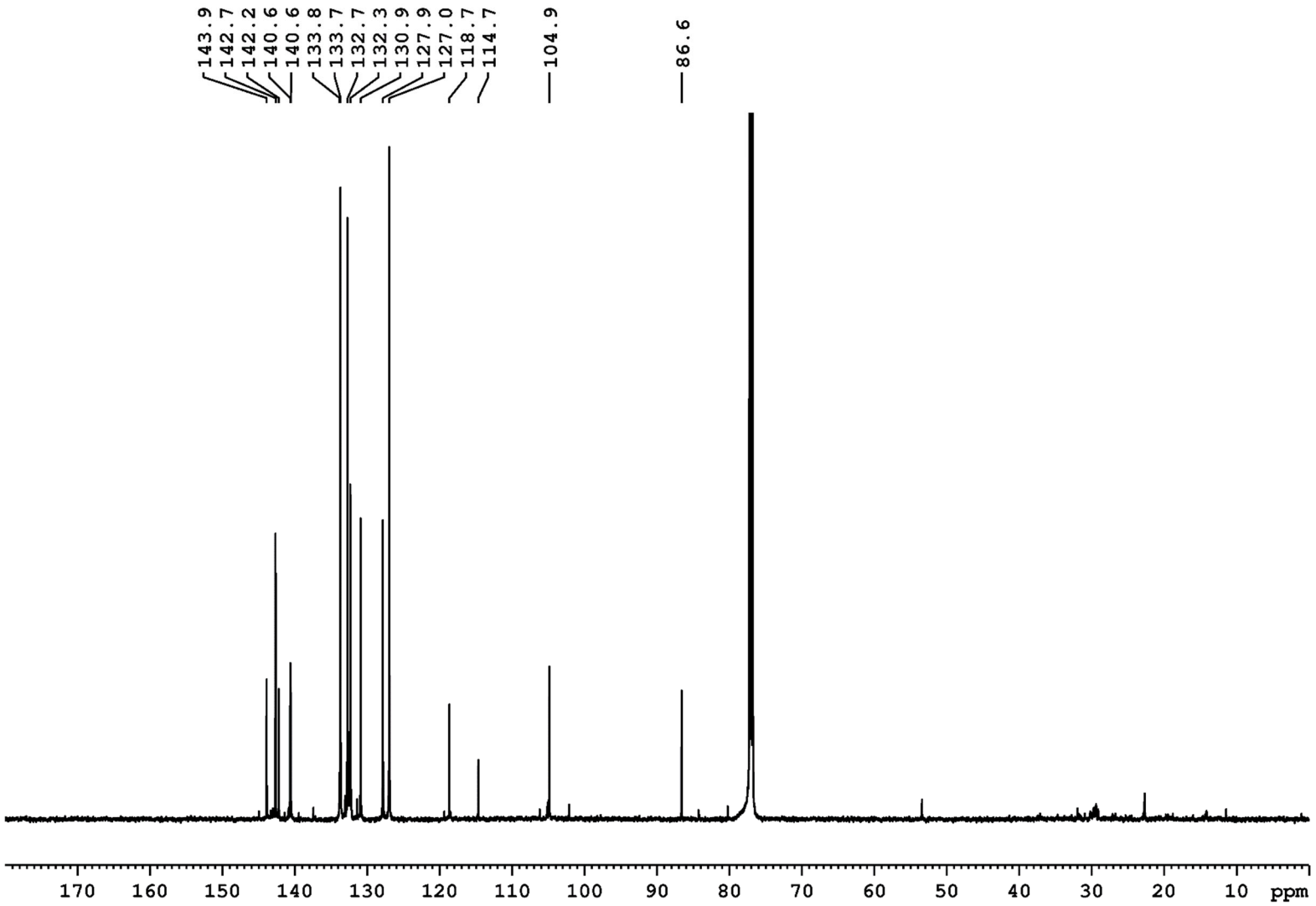

Figure S3. ^{13}C NMR spectrum of *Ni(II) 5-(2-iodoethenyl)-10,20-diphenylporphyrin (7)* in $CDCl_3$.

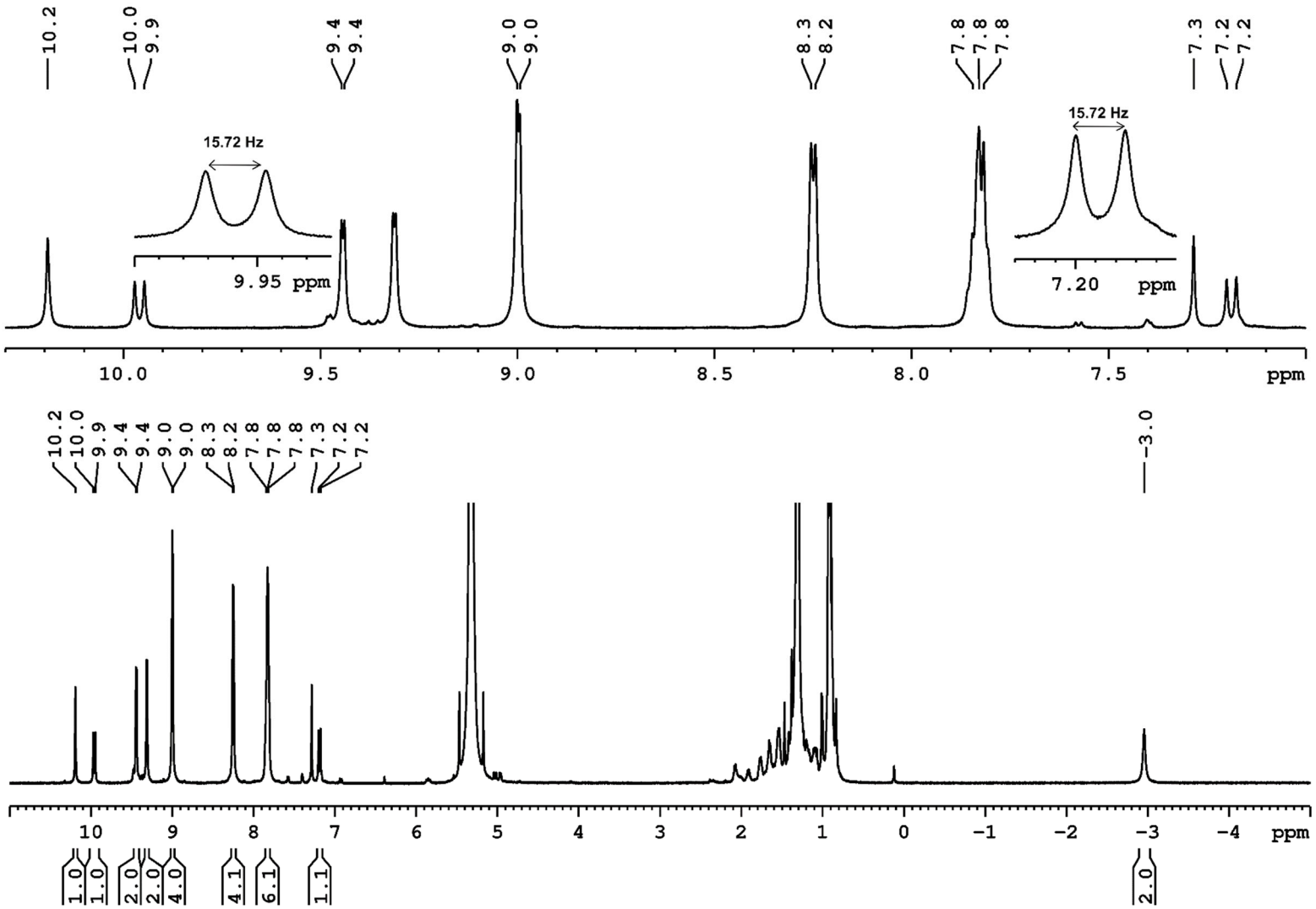

Figure S4. ^{1}H NMR spectrum of *5-(2-iodoethenyl)-10,20-diphenylporphyrin (**8**)* in $CDCl_3$.

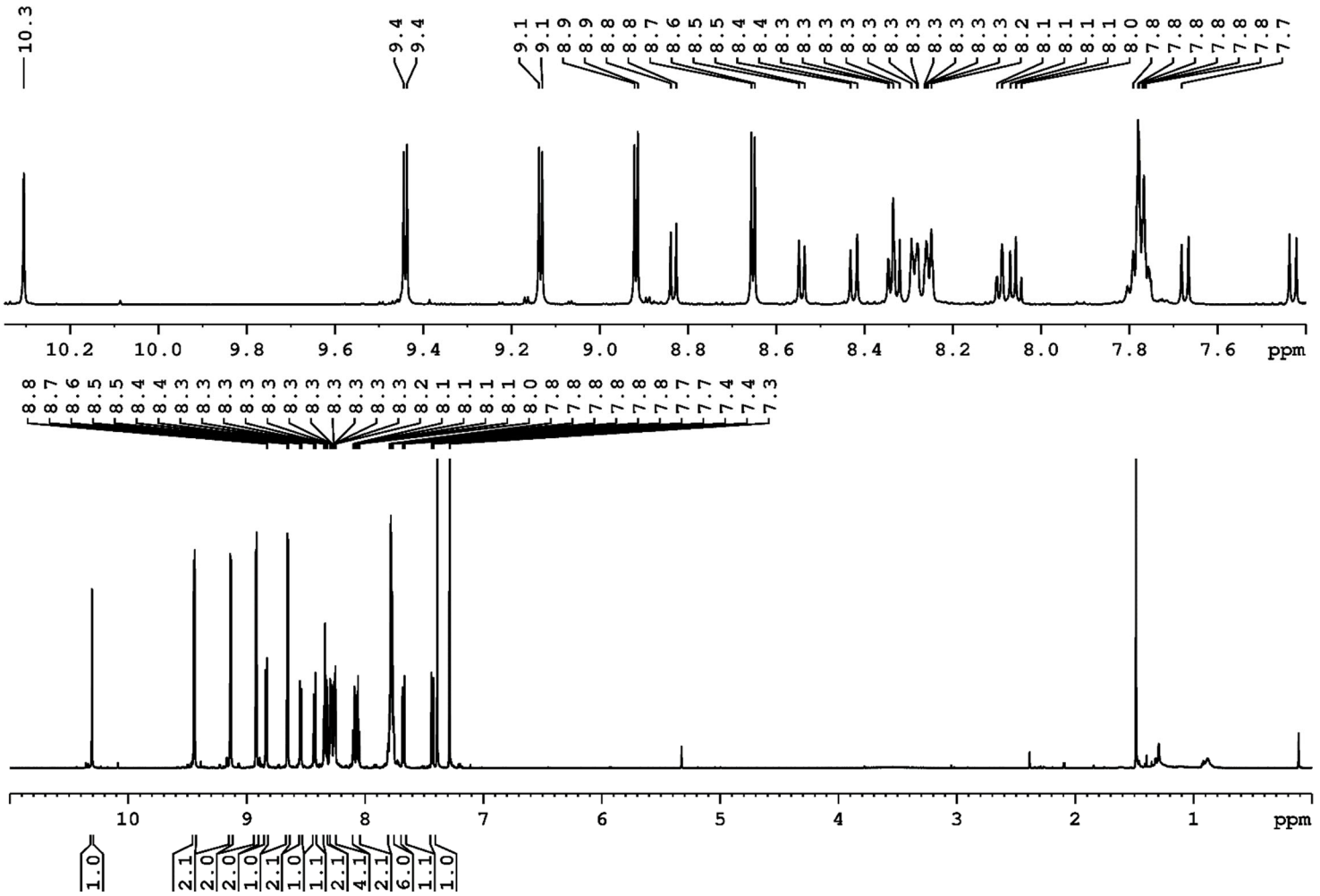

Figure S5. ^{1}H NMR spectrum of *Zn(II) 5-(pyrene-1-yl)-10,20-diphenylporphyrin (**11**)* in $CDCl_3$.

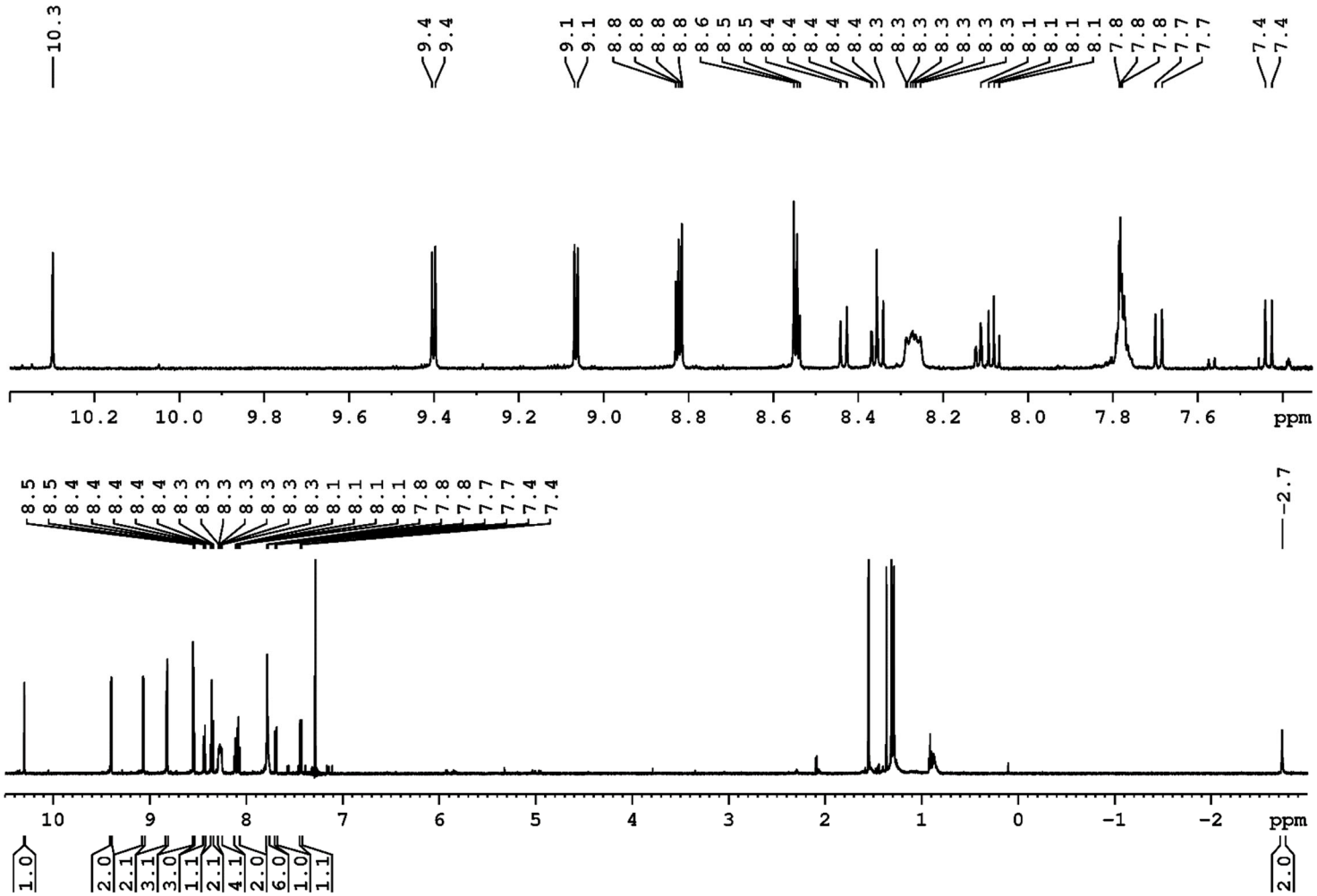

Figure S6. ^{1}H NMR spectrum of *5-(pyrene-1-yl)-10,20-diphenylporphyrin (**12**)* in $CDCl_3$.

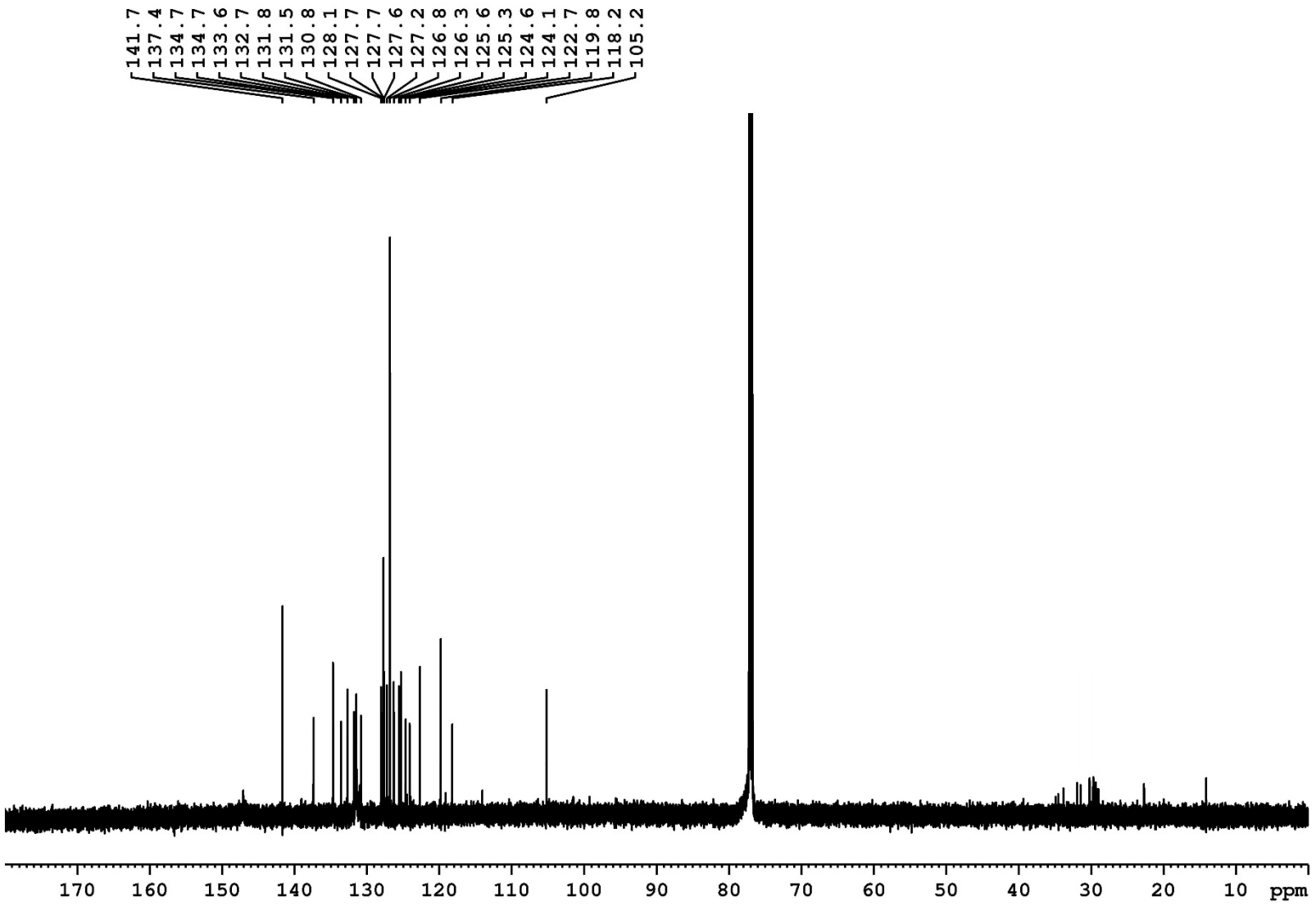

Figure S7. ^{13}C NMR spectrum of *5-(pyrene-1-yl)-10,20-diphenylporphyrin (**12**)* in $CDCl_3$.

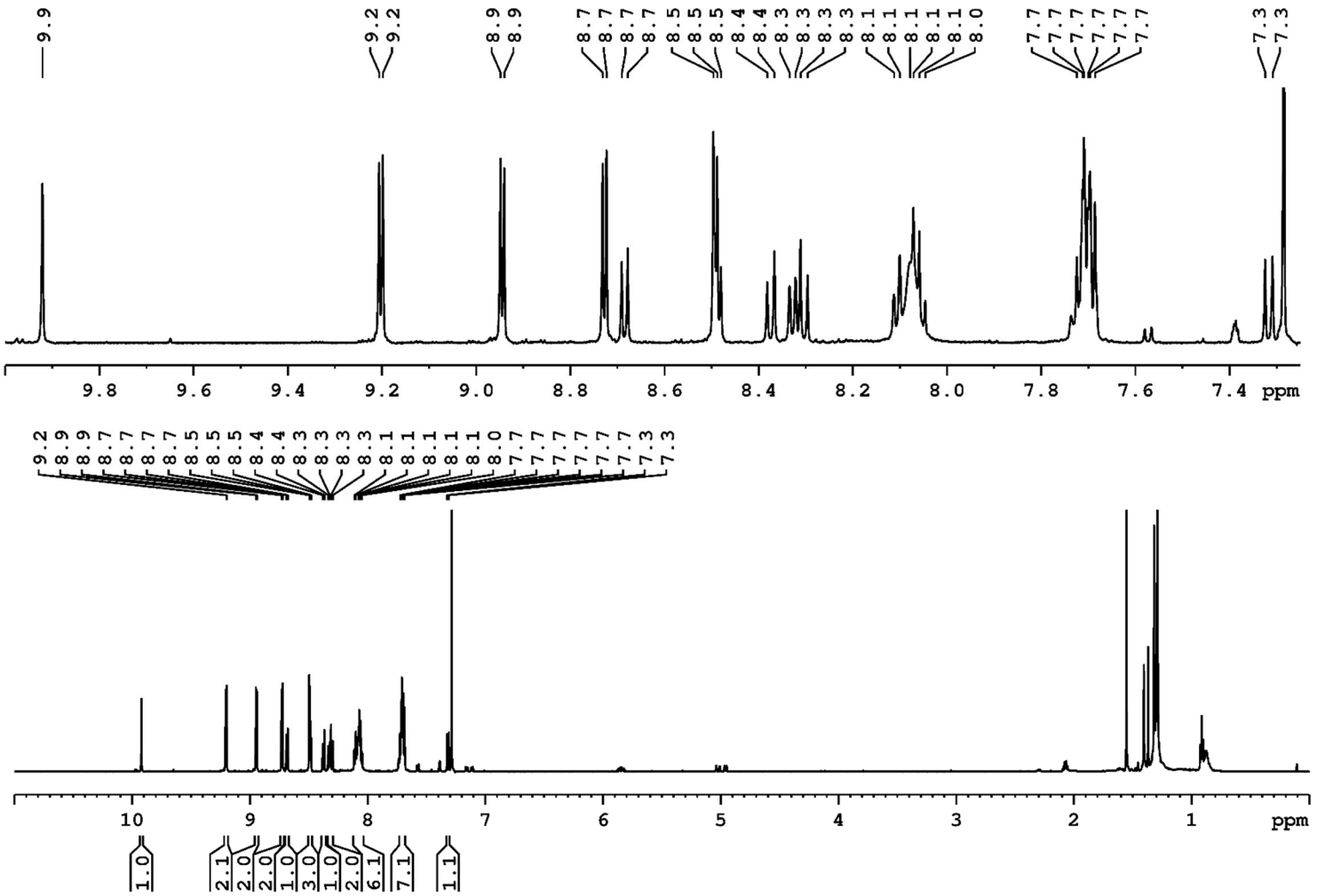

Figure S8. ^{1}H NMR spectrum of *Ni(II) 5-(pyrene-1-yl)-10,20-diphenylporphyrin* ***(13)*** in $CDCl_3$.

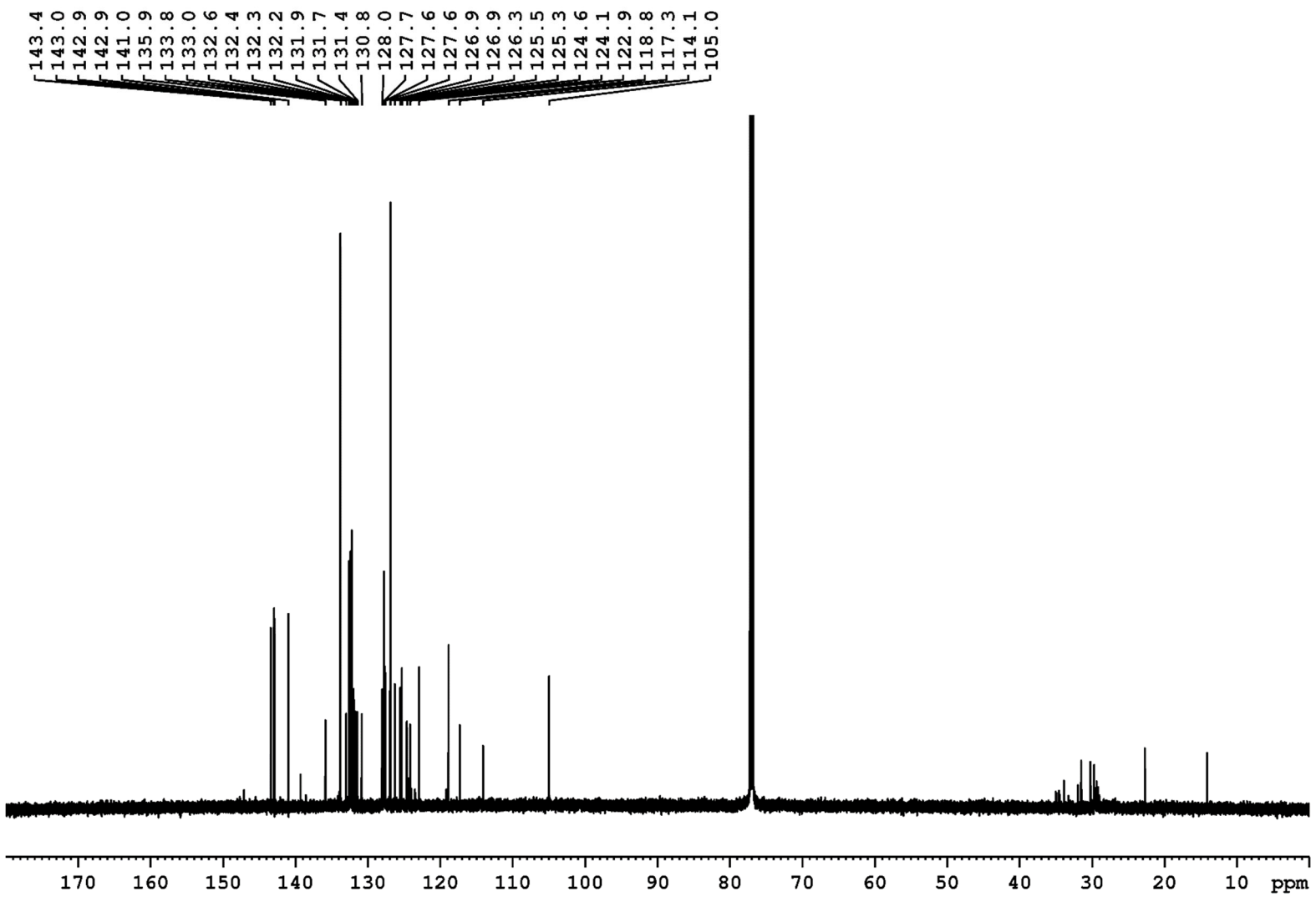

Figure S9. ^{13}C NMR spectrum of *Ni(II) 5-(pyrene-1-yl)-10,20-diphenylporphyrin (**13**)* in $CDCl_3$.

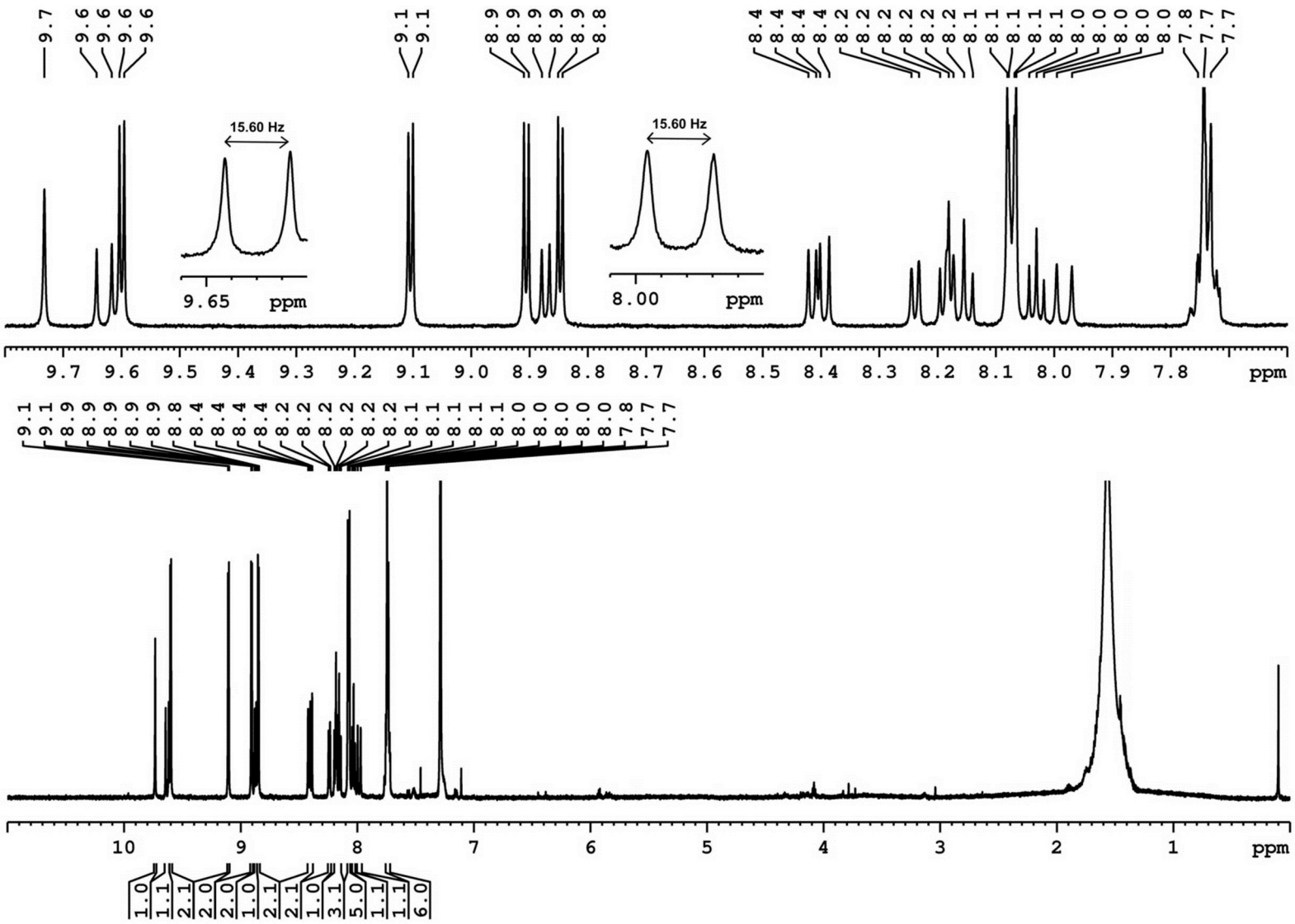

Figure S10. ^{1}H NMR spectrum of *Ni(II) 5-(2-(pyrene-1-yl)ethenyl)-10,20-diphenylporphyrin* ***(14)*** in $CDCl_3$.

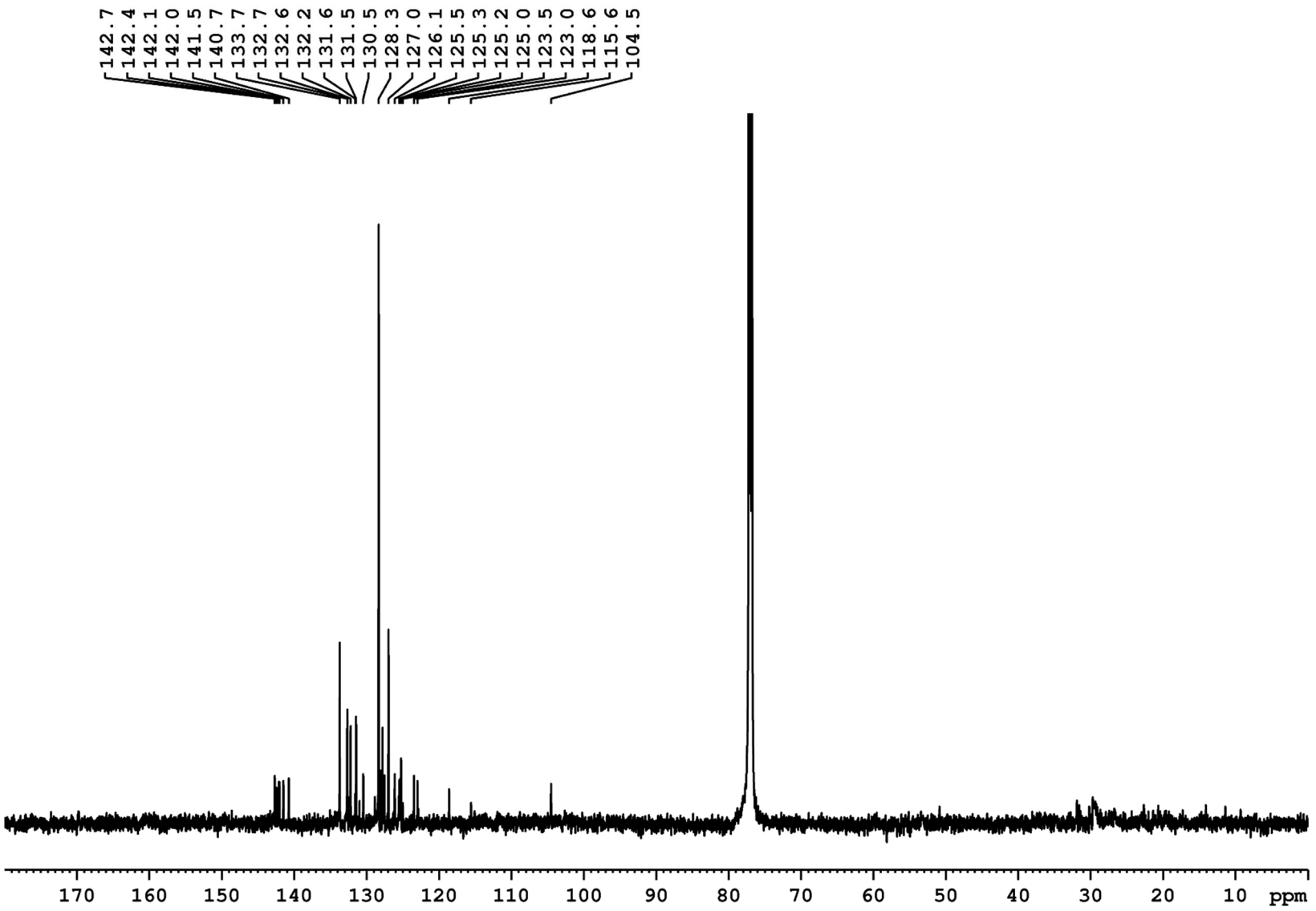

Figure S11. ^{13}C NMR spectrum of *Ni(II) 5-(2-(pyrene-1-yl)ethenyl)-10,20-diphenylporphyrin (**14**)* in $CDCl_3$.

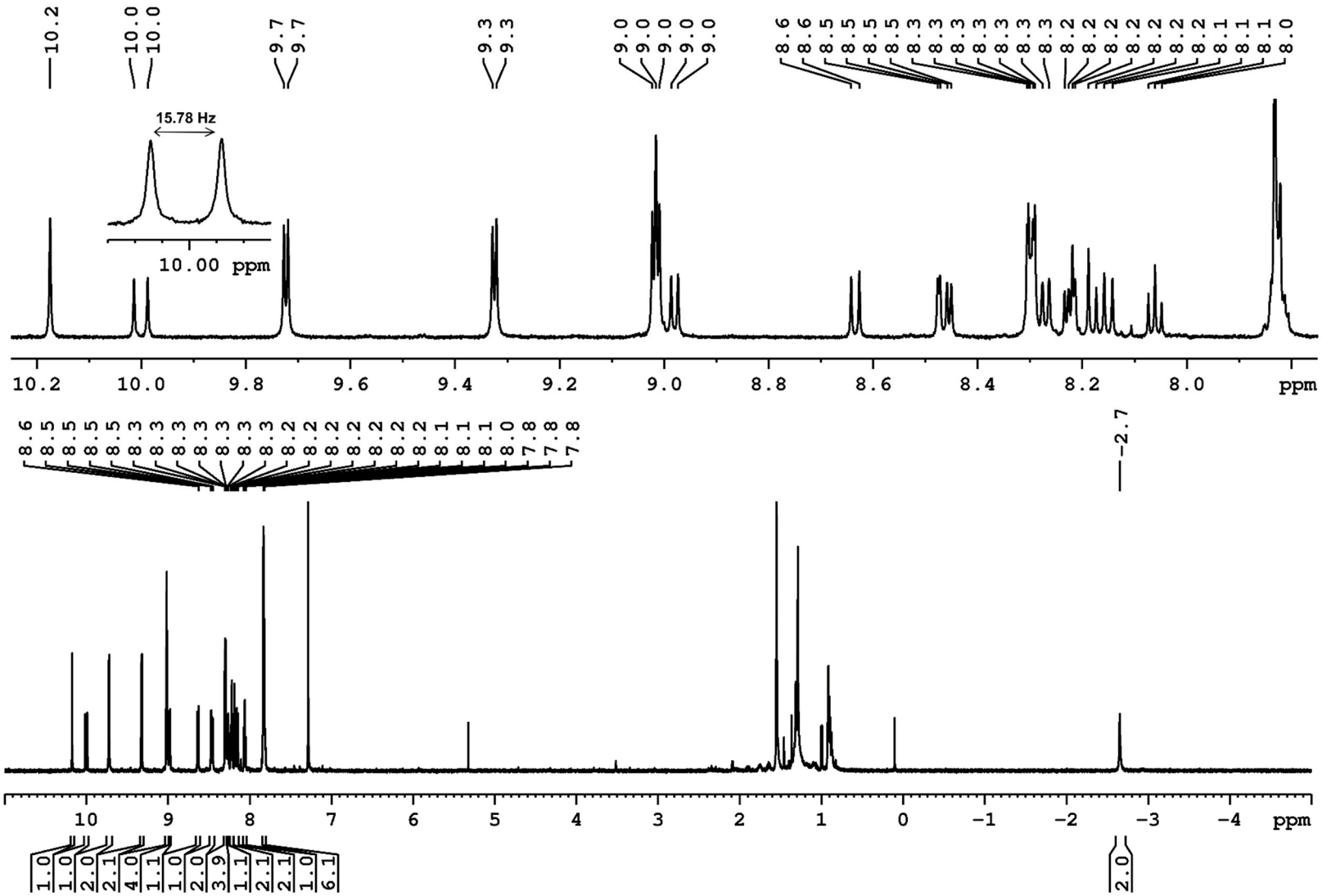

Figure S12. ^{1}H NMR spectrum of *5-(2-(pyrene-1-yl)ethenyl)-10,20-diphenylporphyrin* ***(15)*** in $CDCl_3$.

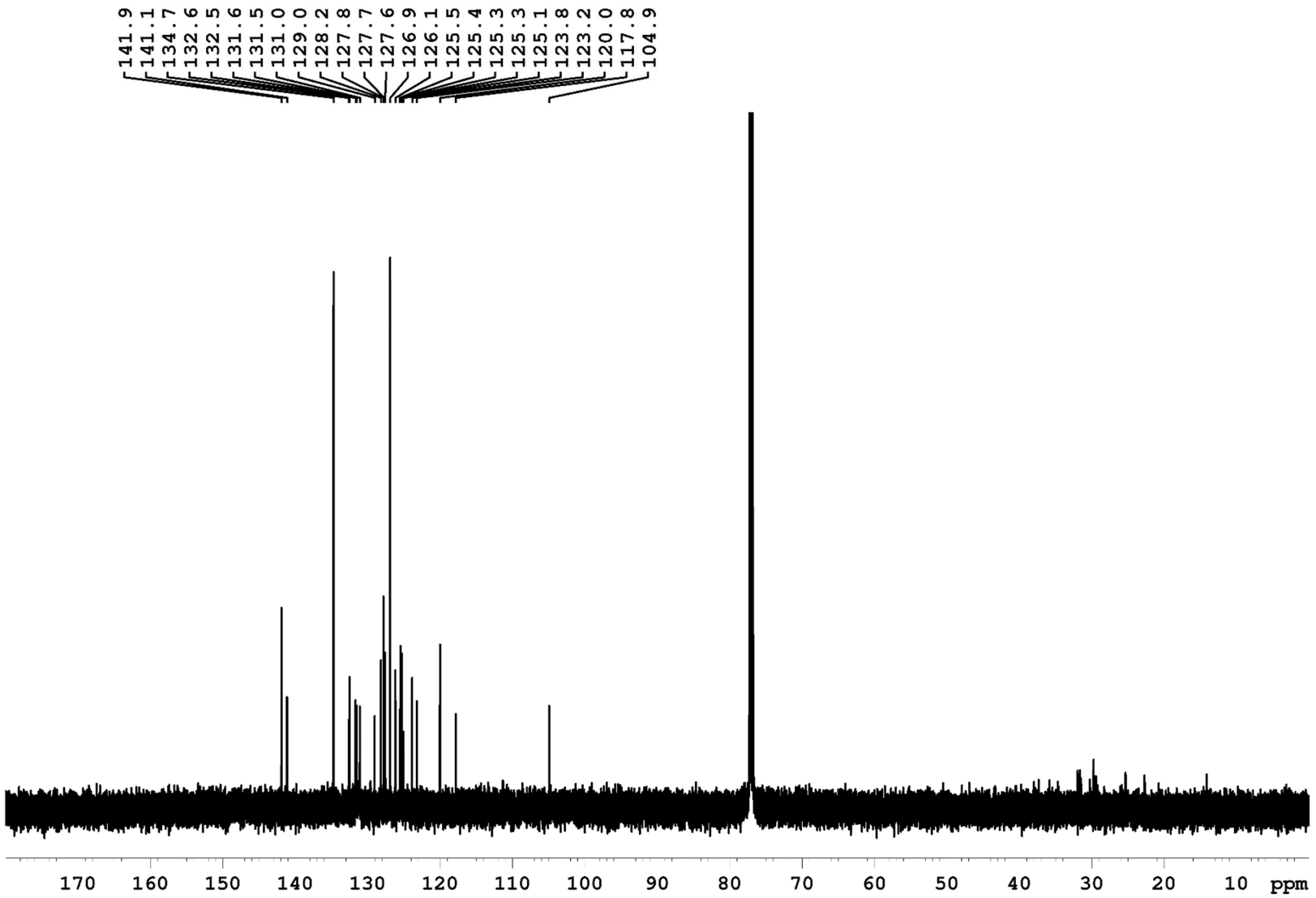

Figure S13. ^{13}C NMR spectrum of *5-(2-(pyrene-1-yl)ethenyl)-10,20-diphenylporphyrin **(15)*** in $CDCl_3$.

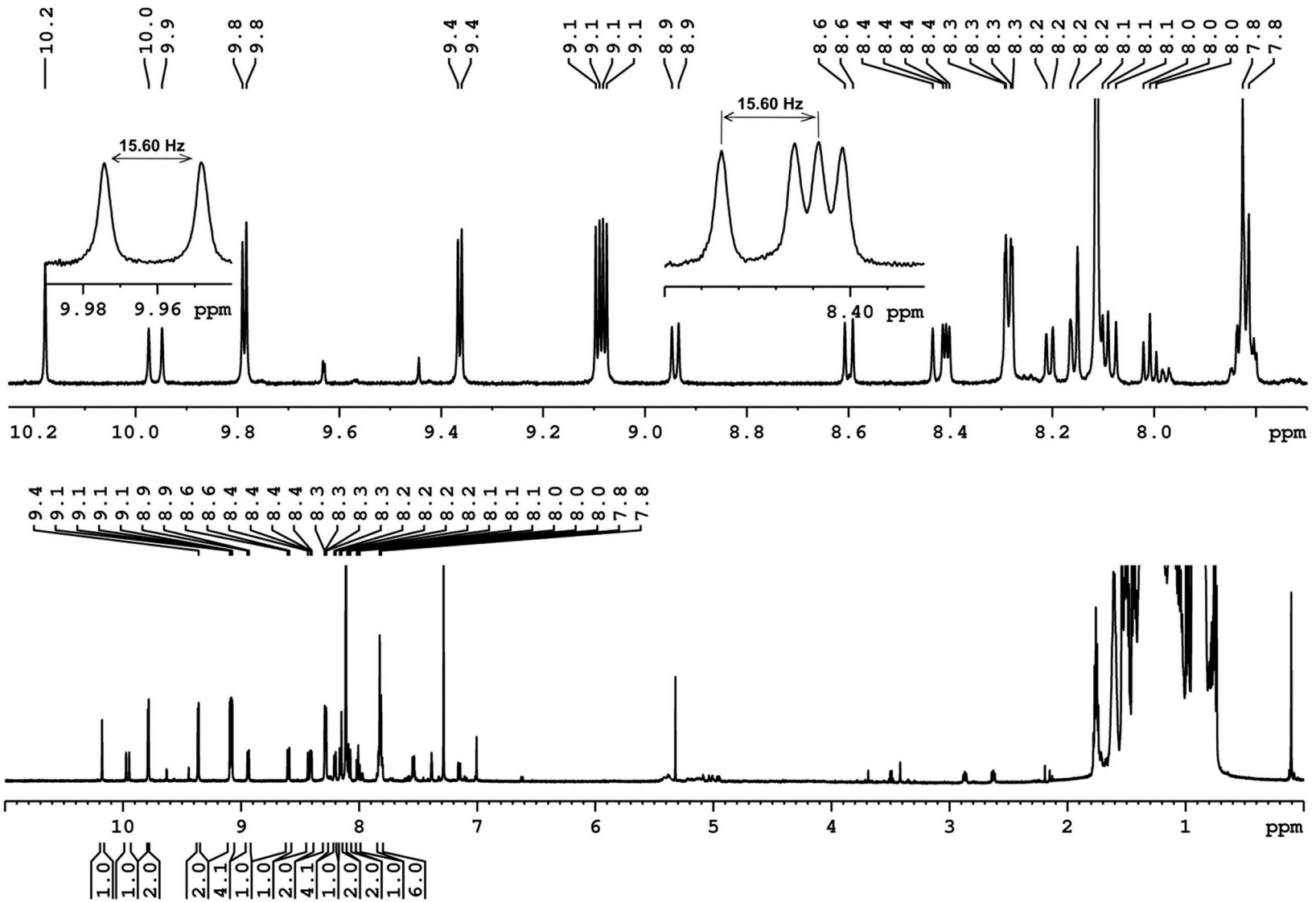

Figure S14. ^{1}H NMR spectrum of *Zn(II) 5-(2-(pyrene-1-yl)ethenyl)-10,20-diphenylporphyrin (**16**)* in $CDCl_3$.

DFT calculations data

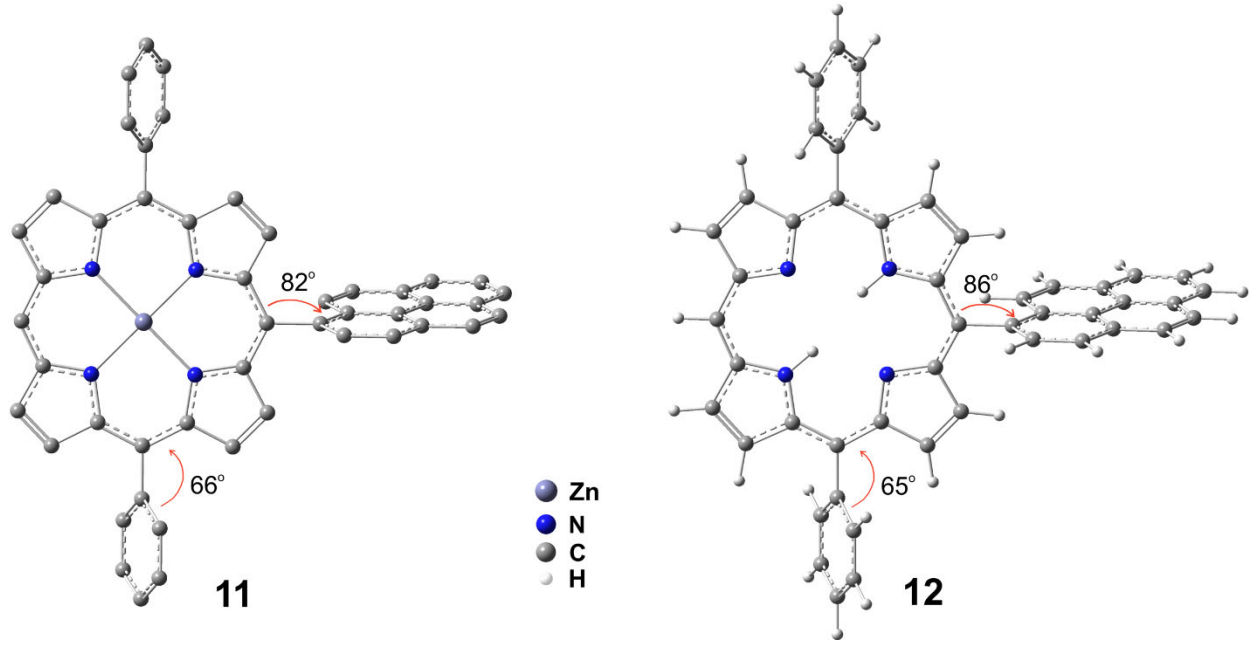

Figure S15. Geometry of the dyads **11** and **12** optimized by the DFT (B3LYP/6-31G(d,p)). Hydrogen atoms in **11** are omitted for clarity.

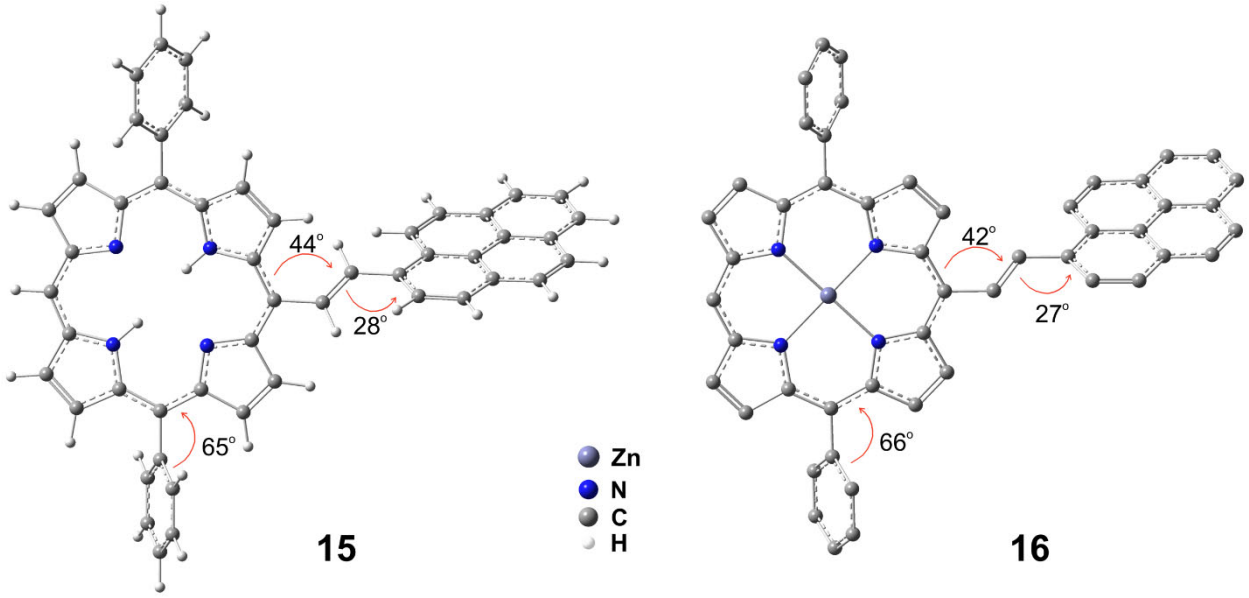

Figure S16. Geometry of the dyads **15** and **16** optimized by the DFT (B3LYP/6-31G(d,p)). Hydrogen atoms in **16** are omitted for clarity.

Table S1. Cartesian coordinates and energy of the dyad **11** in CH_2Cl_2.
RB3LYP/(6-31G(d,p) for C,H,N; LanL2DZ for Zn) E= -2130.731793 a.u., G = -2130.182569 a.u.

Atom	x	y	z
C	2.654339	-5.49924	-1.117
C	2.824692	-4.72912	0.045488
C	3.18483	-5.38378	1.235062
C	3.368465	-6.76745	1.261832
C	3.196225	-7.5215	0.098708
C	2.838841	-6.88274	-1.09105
H	2.382984	-5.00608	-2.04581
H	3.312685	-4.80257	2.143551
H	2.70706	-7.46015	-2.00168
C	-1.55904	2.254767	-0.83724
C	-0.7558	3.342734	-0.66513
C	0.567102	2.851189	-0.33344
N	0.542268	1.476489	-0.31958
C	-0.73923	1.081513	-0.61968
C	0.145889	-3.60045	-0.39535
C	-0.91511	-2.7694	-0.60048
C	-0.40883	-1.41354	-0.55593
N	0.945598	-1.44577	-0.32596
C	1.319277	-2.76517	-0.22985
C	-1.1965	-0.25186	-0.7131
C	5.913696	-1.82032	0.623808
C	5.119552	-2.91641	0.452168
C	3.765741	-2.43441	0.241073
N	3.769636	-1.06242	0.27609
C	5.060181	-0.65945	0.508926
C	2.628336	-3.24386	0.016914
C	4.163703	4.020636	0.4595
C	5.220776	3.179204	0.650265
C	4.722136	1.832493	0.486895
N	3.382354	1.873743	0.19517
C	3.006886	3.193502	0.164562
C	1.699179	3.6661	-0.09257
C	5.489619	0.668702	0.616229
H	-2.60734	2.245588	-1.09845
H	-1.03075	4.382398	-0.76329
H	0.134322	-4.67935	-0.35072
H	-1.94759	-3.04657	-0.75648
H	6.980805	-1.7937	0.803305
H	5.419197	-3.95395	0.46226
H	4.16264	5.099023	0.517875
H	6.243631	3.440035	0.8898
C	2.095243	5.94499	-1.10431
C	1.496223	5.150493	-0.11263
C	0.704147	5.78066	0.861607
C	0.517102	7.163947	0.845285

C	1.118221	7.94239	-0.14663
C	1.907684	7.328267	-1.1217
H	2.703948	5.471189	-1.86885
H	0.240464	5.180403	1.638897
H	2.375204	7.924703	-1.89998
H	3.64169	-7.25585	2.192875
H	3.339245	-8.59795	0.119271
H	6.545207	0.813797	0.827466
H	-0.09498	7.632972	1.610393
H	0.972487	9.018597	-0.15975
C	-2.65012	-0.45563	-1.03919
C	-3.654	-0.38221	-0.04257
C	-3.01867	-0.72712	-2.36392
C	-5.02382	-0.57659	-0.41147
C	-3.35273	-0.1279	1.342609
C	-4.34838	-0.91671	-2.72894
H	-2.24192	-0.7844	-3.12082
C	-6.05161	-0.50557	0.579122
C	-5.37162	-0.84442	-1.77124
C	-4.33375	-0.06196	2.285289
H	-2.31573	0.010834	1.62851
H	-4.60244	-1.12074	-3.76554
C	-5.71732	-0.24437	1.943112
C	-7.41974	-0.69664	0.21008
C	-6.75571	-1.03261	-2.11311
H	-4.08031	0.130306	3.324545
C	-6.74376	-0.17806	2.900426
C	-8.41224	-0.62084	1.201831
C	-7.73363	-0.96144	-1.16817
H	-7.00633	-1.2347	-3.15109
C	-8.07529	-0.36414	2.530616
H	-6.48776	0.020338	3.937712
H	-9.45201	-0.76566	0.921108
H	-8.77541	-1.1056	-1.44196
H	-8.85628	-0.30944	3.283344
Zn	2.163703	0.212396	-0.05923

Table S2. Cartesian coordinates and energy of the dyad **12** in CH_2Cl_2.
RB3LYP/(6-31G(d,p) for C,H,N; LanL2DZ for Zn) E= -2066.286662 a.u., G = -2065.715027 a.u.

Atom	x	y	z
C	2.507878	-5.59959	-1.17619
C	2.740629	-4.86034	-0.00473
C	3.093854	-5.55168	1.165682
C	3.20919	-6.94256	1.165116
C	2.9749	-7.66604	-0.00596
C	2.624008	-6.99008	-1.17658
H	2.242996	-5.07728	-2.09041
H	3.266827	-4.99427	2.081292
H	2.444436	-7.54417	-2.09321

C	-1.26421	2.357621	-0.84398
C	-0.42767	3.42799	-0.66989
C	0.873571	2.926676	-0.33538
N	0.77424	1.552761	-0.32978
C	-0.50893	1.155906	-0.63162
C	0.133215	-3.56307	-0.41566
C	-0.86566	-2.66877	-0.61183
C	-0.25338	-1.34556	-0.55202
N	1.091746	-1.44224	-0.32081
C	1.354922	-2.7843	-0.24408
C	-0.99879	-0.15808	-0.71715
C	5.950241	-2.04497	0.640185
C	5.126097	-3.12451	0.452645
C	3.794667	-2.63307	0.2314
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C	2.621296	-3.36859	-0.00674
C	4.50316	3.862658	0.50906
C	5.491373	2.954682	0.705737
C	4.885028	1.643635	0.519321
N	3.559123	1.752825	0.213574
C	3.300199	3.094807	0.191616
C	2.039476	3.671523	-0.08041
C	5.612204	0.455957	0.647944
H	-2.3109	2.38218	-1.10599
H	-0.67573	4.473502	-0.76795
H	0.060227	-4.63975	-0.37807
H	-1.91479	-2.87052	-0.7708
H	7.014304	-2.05212	0.831905
H	5.400645	-4.16807	0.461726
H	4.565642	4.938765	0.575118
H	6.527884	3.134238	0.960996
C	2.592225	5.921215	-1.07615
C	1.917574	5.162697	-0.10537
C	1.126183	5.834968	0.84045
C	1.013917	7.225809	0.817109
C	1.689813	7.968564	-0.15309
C	2.479101	7.31183	-1.09967
H	3.199914	5.413986	-1.81926
H	0.606877	5.262443	1.60301
H	3.004399	7.880998	-1.86097
H	3.477256	-7.46005	2.08152
H	3.064762	-8.7482	-0.00642
H	6.669877	0.560112	0.869736
H	0.401919	7.728197	1.560424
H	1.602256	9.050762	-0.17144
C	-2.46087	-0.29433	-1.04726
C	-3.45569	-0.2448	-0.04114
C	-2.84263	-0.47226	-2.38325
C	-4.83258	-0.37126	-0.41224

C	-3.13969	-0.07814	1.35377
C	-4.17937	-0.5963	-2.74979
H	-2.07152	-0.51053	-3.14674
C	-5.8527	-0.32219	0.587092
C	-5.19492	-0.54756	-1.78291
C	-4.11372	-0.03276	2.304331
H	-2.09768	0.009116	1.641158
H	-4.4446	-0.73079	-3.79468
C	-5.50377	-0.15001	1.961236
C	-7.22779	-0.44555	0.216318
C	-6.58588	-0.66977	-2.12603
H	-3.84936	0.09291	3.35081
C	-6.52303	-0.10354	2.926846
C	-8.2125	-0.39248	1.21673
C	-7.55624	-0.62057	-1.17251
H	-6.84784	-0.80331	-3.17203
C	-7.86131	-0.22324	2.55543
H	-6.2561	0.027111	3.971893
H	-9.25766	-0.48552	0.934837
H	-8.60327	-0.71425	-1.44743
H	-8.6366	-0.18494	3.314751
H	3.068657	-0.6578	0.129439
H	1.564521	0.942433	-0.15021

Table S3. Cartesian coordinates and energy of the dyad **13** in CH_2Cl_2.
RB3LYP/(6-31G(d,p) for C,H,N; LanL2DZ for Zn) E= -2234.451099 a.u., G = -2233.899458 a.u.

Atom	x	y	z
C	2.923068	-5.19091	-1.59869
C	2.894269	-4.65688	-0.30027
C	3.100167	-5.52074	0.787595
C	3.334096	-6.88155	0.581641
C	3.365267	-7.40058	-0.71483
C	3.158581	-6.55144	-1.80442
H	2.765513	-4.53276	-2.44821
H	3.067747	-5.12298	1.797605
H	3.182485	-6.94637	-2.81598
C	-1.44526	2.202495	-1.06062
C	-0.60141	3.265223	-1.00438
C	0.667567	2.769679	-0.53366
N	0.61221	1.398879	-0.35955
C	-0.68307	1.042775	-0.67741
C	0.228308	-3.53805	-0.65359
C	-0.85625	-2.72616	-0.74754
C	-0.38644	-1.37818	-0.55723
N	0.971479	-1.37169	-0.30116
C	1.360953	-2.69546	-0.36253
C	-1.19707	-0.25391	-0.70751
C	5.588576	-1.81816	1.414527
C	4.933788	-2.87474	0.864876

C	3.649358	-2.38631	0.420891
N	3.547103	-1.02814	0.649743
C	4.731546	-0.67448	1.258437
C	2.637267	-3.1973	-0.09333
C	3.968593	3.916028	0.895784
C	4.872346	3.080777	1.472748
C	4.388726	1.742774	1.264934
N	3.181508	1.755019	0.5998
C	2.912847	3.087583	0.362867
C	1.755007	3.592247	-0.23103
C	5.10621	0.610819	1.605989
H	-2.48236	2.186632	-1.361
H	-0.81254	4.296733	-1.24148
H	0.267371	-4.61296	-0.74444
H	-1.88179	-2.99982	-0.94531
H	6.572806	-1.79125	1.862928
H	5.269193	-3.89692	0.777487
H	3.989688	4.994185	0.844678
H	5.794996	3.328031	1.980822
Ni	2.078049	0.188494	0.146187
C	2.457222	5.661787	-1.47489
C	1.661233	5.064371	-0.48438
C	0.794586	5.877188	0.264074
C	0.722191	7.250522	0.024093
C	1.515337	7.833114	-0.96728
C	2.383474	7.034975	-1.71572
H	3.131226	5.043326	-2.06049
H	0.182085	5.42948	1.041125
H	3.002773	7.479515	-2.48945
H	3.486878	-7.53601	1.434958
H	3.547587	-8.45924	-0.87464
H	6.060094	0.745128	2.104271
H	0.049178	7.86491	0.615179
H	1.458352	8.901507	-1.15397
C	-2.65538	-0.44537	-1.00427
C	-3.62798	-0.35679	0.021238
C	-3.06282	-0.71412	-2.31796
C	-5.00935	-0.53982	-0.30747
C	-3.28404	-0.09575	1.395191
C	-4.40444	-0.89206	-2.64312
H	-2.30881	-0.78016	-3.09677
C	-6.00713	-0.45536	0.71211
C	-5.39845	-0.809	-1.65572
C	-4.23698	-0.01633	2.365218
H	-2.23838	0.03728	1.651284
H	-4.69054	-1.09582	-3.67133
C	-5.63114	-0.19029	2.064369
C	-7.38678	-0.63659	0.383781
C	-6.79344	-0.98683	-1.9565
H	-3.95194	0.180954	3.395232

C	-6.62861	-0.11119	3.050822
C	-8.34931	-0.54838	1.403618
C	-7.74267	-0.90429	-0.98361
H	-7.07593	-1.19048	-2.98588
C	-7.97177	-0.28841	2.720808
H	-6.34095	0.090143	4.079194
H	-9.39793	-0.68595	1.153992
H	-8.79308	-1.04099	-1.22643
H	-8.73	-0.22402	3.495669
H	1.564521	0.942433	-0.15021

Table S4. Cartesian coordinates and energy of the dyad **14** in CH_2Cl_2.
RB3LYP/(6-31G(d,p) for C,H,N; LanL2DZ for Zn) E= -2311.857174 a.u., G = -2311.274114 a.u.

Atom	x	y	z
C	4.873921	-4.58034	-1.51989
C	4.60307	-4.15973	-0.20746
C	4.889558	-5.03601	0.852223
C	5.440187	-6.29491	0.605924
C	5.711995	-6.69921	-0.70324
C	5.426144	-5.83861	-1.76558
H	4.655326	-3.9124	-2.34796
H	4.668542	-4.73141	1.870799
H	5.634356	-6.1446	-2.78676
C	-0.83678	1.628268	-1.57183
C	-0.1568	2.807347	-1.55681
C	1.05812	2.581509	-0.82135
N	1.155625	1.244654	-0.47211
C	-0.01458	0.658551	-0.89505
C	1.787436	-3.63235	-0.76841
C	0.552184	-3.07564	-0.88922
C	0.700578	-1.66505	-0.63963
N	2.008571	-1.37881	-0.31099
C	2.686365	-2.58073	-0.37281
C	-0.3219	-0.71447	-0.81732
C	6.283119	-0.9613	2.112309
C	5.994682	-2.08157	1.395924
C	4.729109	-1.84629	0.741247
N	4.289304	-0.56485	1.006276
C	5.235723	-0.01408	1.840304
C	4.005843	-2.81039	0.035039
C	3.751221	4.343315	1.152349
C	4.617537	3.696368	1.978352
C	4.431326	2.287983	1.75176
N	3.422235	2.074396	0.838769
C	2.999157	3.327843	0.453196
C	1.936463	3.59216	-0.41613
C	5.258864	1.304339	2.267052
H	-1.78065	1.415011	-2.04862
H	-0.45256	3.748494	-1.99465

H	2.064409	-4.66806	-0.89492
H	-0.36411	-3.58254	-1.15087
H	7.142069	-0.76467	2.740109
H	6.566178	-2.99476	1.328296
H	3.607631	5.406918	1.03428
H	5.341946	4.118892	2.661921
Ni	2.717466	0.343004	0.272473
C	2.633661	5.66947	-1.64238
C	1.692087	5.004769	-0.83918
C	0.540554	5.701824	-0.43725
C	0.333526	7.023974	-0.83398
C	1.273854	7.671839	-1.6386
C	2.424989	6.990789	-2.04103
H	3.528104	5.141667	-1.96005
H	-0.18793	5.206542	0.197553
H	3.161019	7.486146	-2.66767
H	5.650848	-6.96138	1.437335
H	6.140725	-7.67865	-0.89408
H	6.045234	1.60554	2.950574
H	-0.56023	7.548885	-0.50921
H	1.111685	8.700301	-1.94766
C	-1.69501	-1.18113	-1.00506
H	-1.82078	-2.15815	-1.46038
C	-2.8039	-0.5321	-0.57334
H	-2.66584	0.389844	-0.01739
C	-4.18102	-0.98378	-0.77892
C	-5.22675	-0.59851	0.111643
C	-4.50373	-1.79473	-1.88581
C	-6.56598	-1.03919	-0.14282
C	-4.99794	0.203158	1.284643
C	-5.7967	-2.23052	-2.12719
H	-3.72017	-2.05777	-2.58919
C	-7.63074	-0.66153	0.733917
C	-6.85203	-1.86483	-1.2736
C	-6.01378	0.564177	2.119015
H	-3.98942	0.519676	1.523607
H	-6.00736	-2.84671	-2.99704
C	-7.36641	0.152673	1.876578
C	-8.96794	-1.09816	0.474509
C	-8.20274	-2.28873	-1.51007
H	-5.80707	1.171415	2.996276
C	-8.42654	0.51548	2.725232
C	-9.99677	-0.71017	1.349983
C	-9.21603	-1.92236	-0.67583
H	-8.40144	-2.91397	-2.37641
C	-9.72687	0.088016	2.461192
H	-8.22039	1.134785	3.593971
H	-11.0122	-1.04176	1.150785
H	-10.2339	-2.25097	-0.86744
H	-10.5353	0.377093	3.126236

Table S5. Cartesian coordinates and energy of the dyad **15** in CH_2Cl_2.
RB3LYP/(6-31G(d,p) for C,H,N; LanL2DZ for Zn) E= -2143.692963 a.u., G = -2143.089988 a.u.

Atom	x	y	z
C	4.237085	-5.28363	-1.11596
C	4.306273	-4.53447	0.070109
C	4.710179	-5.18104	1.2496
C	5.035489	-6.53822	1.243099
C	4.964255	-7.27171	0.057039
C	4.564034	-6.64009	-1.12247
H	3.93269	-4.79446	-2.0362
H	4.756715	-4.61746	2.176482
H	4.509243	-7.20183	-2.05032
C	-0.64782	1.96468	-1.2044
C	0.034179	3.141174	-1.03574
C	1.318198	2.837091	-0.48209
N	1.370312	1.465364	-0.34905
C	0.188215	0.888864	-0.75603
C	1.548026	-3.66865	-0.36885
C	0.418361	-2.95098	-0.58273
C	0.809458	-1.54578	-0.56444
N	2.148545	-1.4199	-0.3246
C	2.625029	-2.70149	-0.20992
C	-0.12181	-0.49111	-0.76995
C	6.998705	-1.28067	0.951231
C	6.364238	-2.46666	0.683806
C	4.992897	-2.17643	0.372091
N	4.856423	-0.80982	0.442121
C	6.046495	-0.22244	0.795649
C	3.958984	-3.07832	0.070576
C	4.665668	4.328275	0.682535
C	5.757617	3.588152	0.996732
C	5.383674	2.197168	0.780936
N	4.090284	2.093444	0.355861
C	3.632828	3.378133	0.270228
C	2.339668	3.750442	-0.15664
C	6.278334	1.139897	0.970024
H	-1.62694	1.841686	-1.63792
H	-0.30363	4.132652	-1.29441
H	1.646841	-4.74185	-0.30292
H	-0.58096	-3.33835	-0.71571
H	8.033924	-1.13304	1.226079
H	6.792722	-3.45683	0.701121
H	4.554338	5.401464	0.727469
H	6.724562	3.930208	1.34295
C	2.710999	6.014022	-1.20387
C	2.016222	5.204814	-0.2893
C	1.0104	5.792886	0.495746
C	0.710668	7.150094	0.372359

C	1.409133	7.943349	-0.5403
C	2.409788	7.370689	-1.32838
H	3.483096	5.570986	-1.8253
H	0.471064	5.18236	1.213521
H	2.954151	7.978484	-2.04512
H	5.33951	-7.0225	2.166414
H	5.217854	-8.32757	0.052037
H	7.28435	1.404413	1.280438
H	-0.06562	7.587765	0.993078
H	1.17532	8.999365	-0.6369
C	-1.51496	-0.88076	-1.04719
H	-1.64861	-1.74712	-1.68824
C	-2.6173	-0.29743	-0.52314
H	-2.4742	0.49962	0.199924
C	-3.99967	-0.66724	-0.83944
C	-5.05607	-0.44871	0.092614
C	-4.31286	-1.22734	-2.09356
C	-6.39748	-0.79638	-0.27003
C	-4.83713	0.089615	1.408999
C	-5.6083	-1.57474	-2.44165
H	-3.51893	-1.35986	-2.82133
C	-7.47338	-0.58064	0.646583
C	-6.67458	-1.36624	-1.55062
C	-5.86337	0.296062	2.281616
H	-3.82785	0.325515	1.724965
H	-5.81134	-1.99538	-3.42253
C	-7.21816	-0.02416	1.936193
C	-8.8127	-0.92249	0.279593
C	-8.02783	-1.70032	-1.8925
H	-5.66411	0.705092	3.268386
C	-8.28932	0.182858	2.821894
C	-9.85251	-0.69673	1.197313
C	-9.05148	-1.48782	-1.01924
H	-8.21962	-2.1302	-2.87182
C	-9.59143	-0.14962	2.452788
H	-8.09034	0.606007	3.802556
H	-10.8696	-0.95569	0.916272
H	-10.0712	-1.74554	-1.29175
H	-10.4084	0.017018	3.148391
H	2.19039	0.966116	-0.02254
H	3.993912	-0.32056	0.227043

Table S6. Cartesian coordinates and energy of the dyad **16** in CH_2Cl_2.
RB3LYP/(6-31G(d,p) for C,H,N; LanL2DZ for Zn) E = -2208.136401 a.u., G = -2207.555992 a.u.

Atom	x	y	z
C	4.006218	-5.3431	-1.01395
C	4.095851	-4.54336	0.137442
C	4.515884	-5.14165	1.33707
C	4.836475	-6.49953	1.384251

C	4.744363	-7.28337	0.231754
C	4.328524	-6.70059	-0.9677
H	3.689114	-4.89289	-1.95003
H	4.582061	-4.53772	2.237259
H	4.257977	-7.30124	-1.87005
C	-0.9019	1.951413	-1.08615
C	-0.20589	3.111506	-0.91517
C	1.101516	2.755612	-0.41089
N	1.177341	1.385774	-0.28987
C	-0.03604	0.866549	-0.67271
C	1.322555	-3.70079	-0.29759
C	0.178965	-2.98886	-0.51084
C	0.54106	-1.58772	-0.51555
N	1.890624	-1.47418	-0.2961
C	2.401509	-2.74634	-0.16642
C	-0.37496	-0.51458	-0.70183
C	6.86684	-1.33412	0.724756
C	6.192776	-2.50603	0.539938
C	4.800581	-2.16516	0.309125
N	4.662599	-0.7997	0.338933
C	5.899904	-0.26775	0.596997
C	3.752116	-3.08573	0.08701
C	4.524012	4.291609	0.522786
C	5.654527	3.563874	0.753527
C	5.303071	2.172626	0.580091
N	3.974993	2.074289	0.249992
C	3.469498	3.34885	0.193176
C	2.136833	3.682919	-0.13695
C	6.186375	1.09701	0.722816
H	-1.89469	1.844297	-1.49427
H	-0.53805	4.11317	-1.14404
H	1.421273	-4.77344	-0.22248
H	-0.81702	-3.39011	-0.62848
H	7.922315	-1.1977	0.922194
H	6.597331	-3.50723	0.555124
H	4.41039	5.364258	0.574654
H	6.637161	3.929061	1.023148
C	2.396844	5.970083	-1.17687
C	1.791099	5.13747	-0.22065
C	0.849796	5.702116	0.6567
C	0.526805	7.057988	0.582897
C	1.136931	7.874456	-0.37237
C	2.072326	7.325639	-1.25275
H	3.118246	5.54653	-1.86933
H	0.377261	5.072465	1.404763
H	2.547243	7.951118	-2.00325
H	5.153917	-6.94493	2.322802
H	4.994294	-8.33971	0.268107
H	7.215847	1.350595	0.95888
H	-0.19891	7.476469	1.27443

H	0.88494	8.929314	-0.43078
C	-1.76819	-0.90259	-0.97446
H	-1.89942	-1.77732	-1.60588
C	-2.87791	-0.31494	-0.46915
H	-2.74645	0.488768	0.248733
C	-4.25465	-0.68621	-0.80936
C	-5.3321	-0.45428	0.095401
C	-4.54231	-1.25879	-2.06469
C	-6.6667	-0.79998	-0.29457
C	-5.14134	0.098061	1.410567
C	-5.83085	-1.60627	-2.43848
H	-3.73292	-1.40059	-2.7736
C	-7.76302	-0.56793	0.593802
C	-6.91688	-1.38336	-1.57484
C	-6.18697	0.319816	2.256648
H	-4.13812	0.332797	1.746731
H	-6.0129	-2.03697	-3.41937
C	-7.53531	0.002752	1.882693
C	-9.09552	-0.90685	0.198937
C	-8.26359	-1.71468	-1.94497
H	-6.00901	0.739358	3.243277
C	-8.62632	0.226651	2.740165
C	-10.1559	-0.66412	1.0889
C	-9.30683	-1.48645	-1.09871
H	-8.43432	-2.15489	-2.92382
C	-9.92157	-0.103	2.343881
H	-8.4483	0.66087	3.720215
H	-11.1676	-0.92072	0.786598
H	-10.3214	-1.7418	-1.39248
H	-10.7541	0.076883	3.017689
Zn	2.926464	0.298155	0.003344