Supporting Information

Electron beam-induced demetallation of Fe, Co, Ni, Cu, Zn, Pd, and Pt metalloporphyrins: Insights in e-beam chemistry and metal cluster formations

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This PDF file includes:

Captions for Supporting Video S1 to S3, Supplementary Synthetic Details, Supplementary Computational Details, XYZ Coordinates, Spectral Appendix, Supplementary Text, Supporting Figure S1 to S49, Supporting Table S1 to S9, Supplementary References.

Other Supplementary Materials for this manuscript include the following:

Supporting Video S1 to S3

Content

1. Caption for Videos

Supporting Video S1: Single Pt atom dynamics.

80 kV, magnification 2,000,000x, t_{exp} = 40 ms, drift corrected, gaussian blurred, bandpass filtered, and contrast corrected. Video displayed at 25 fps, 1-909 frames. The video displays the motion 5 times faster than the actual recording.

Supporting Video S2: Dynamics of coalescence of three amorphous Pt clusters.

80 kV, magnification 2,000,000x, t_{exp} = 200 ms, drift corrected, contrast corrected. Video displayed at 5 fps, 1-523 frames. The video displays the motion 5 times faster than the actual recording.

Supporting Video S3: Dynamics of atomic rearrangements in a crystalline Ni cluster.

80 kV, magnification 2,000,000x, t_{exp} = 200 ms, drift corrected, gaussian blurred, and contrast corrected. Video displayed at 5 fps, 1-289 frames. The video displays the motion 5 times faster than the actual recording.

2. Electron Microscopy Section

2.1 Graphene Grid Preparation

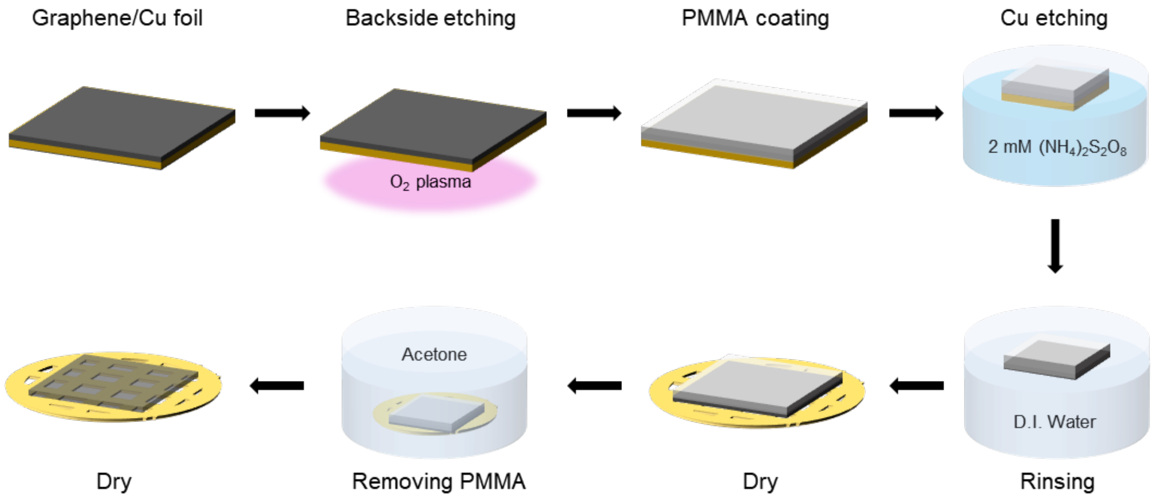


Figure S1. Sequence of the preparation steps for the preparation of graphene-coated TEM grids.

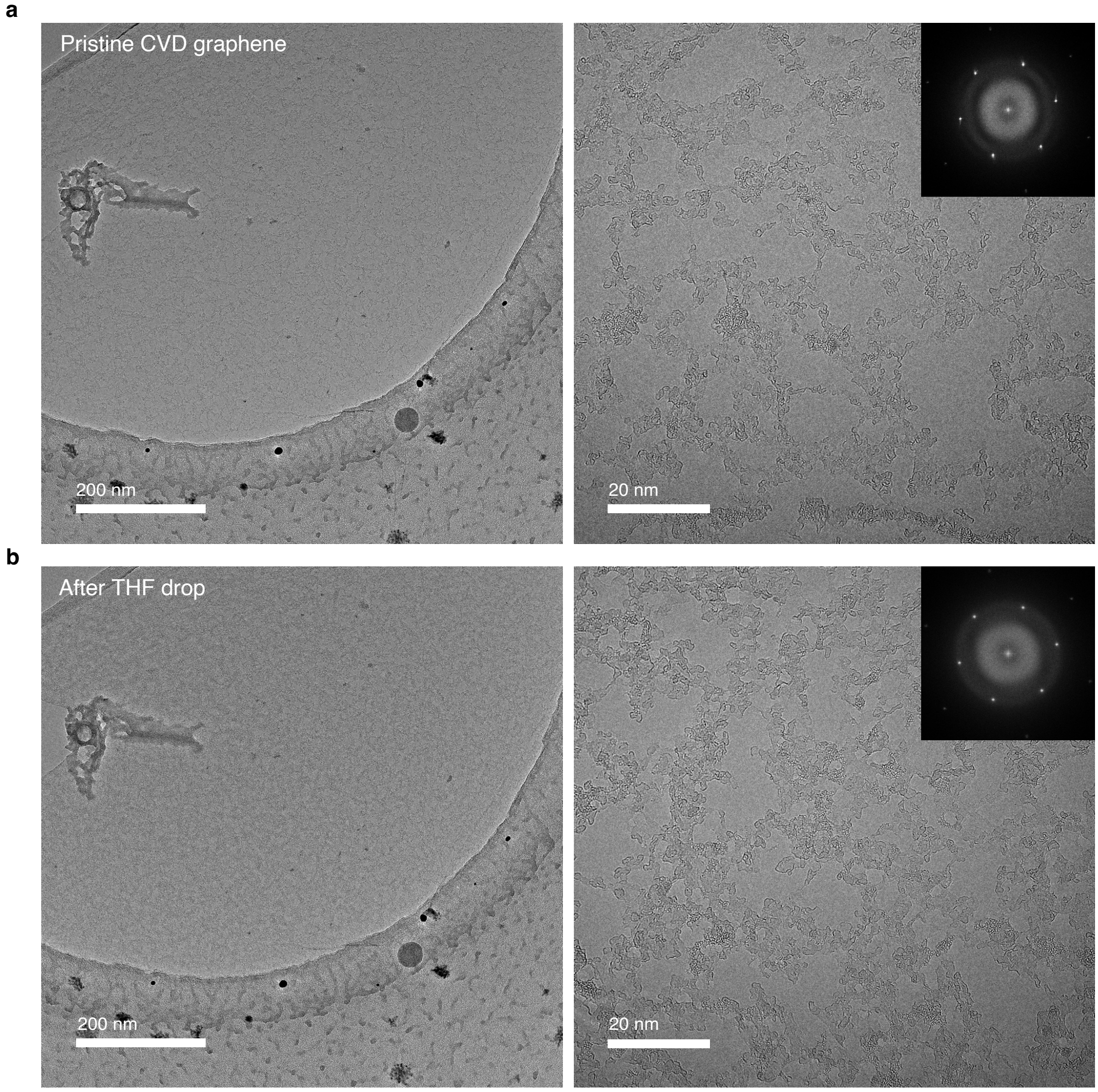


Figure S2. Low (left) and high (right) magnification TEM images of a) as synthesized CVD graphene, and b) THF drop-casted graphene. The TEM images in a) and b) show the same region for comparison. The THF drop-casted graphene grid was dried in vacuum (10^{-3} mbar) for 12 h before subjecting to TEM imaging. Considering the fact that solvent molecules show only little increase in amorphous carbon formation, the contribution of MTPP molecules to the formation of amorphous carbon, which are subjected in a mM concentration in the demetallation experiments, is neglectable.

2.2 Elastic Scattering Cross-Section

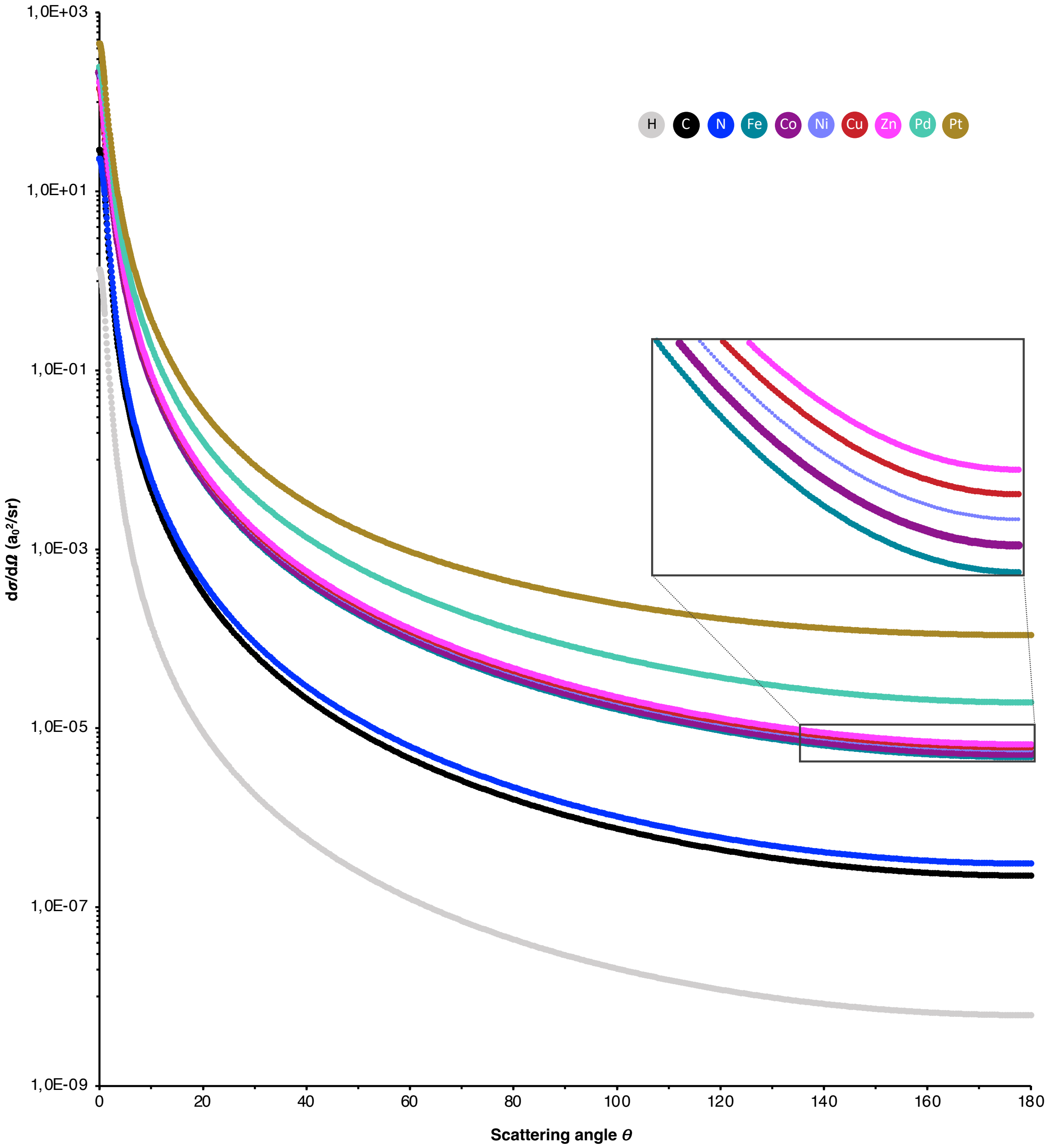


Figure S3. Elastic electron scattering cross-section at 80 keV.

2.3 Metal Clusters Versus Metal Carbides

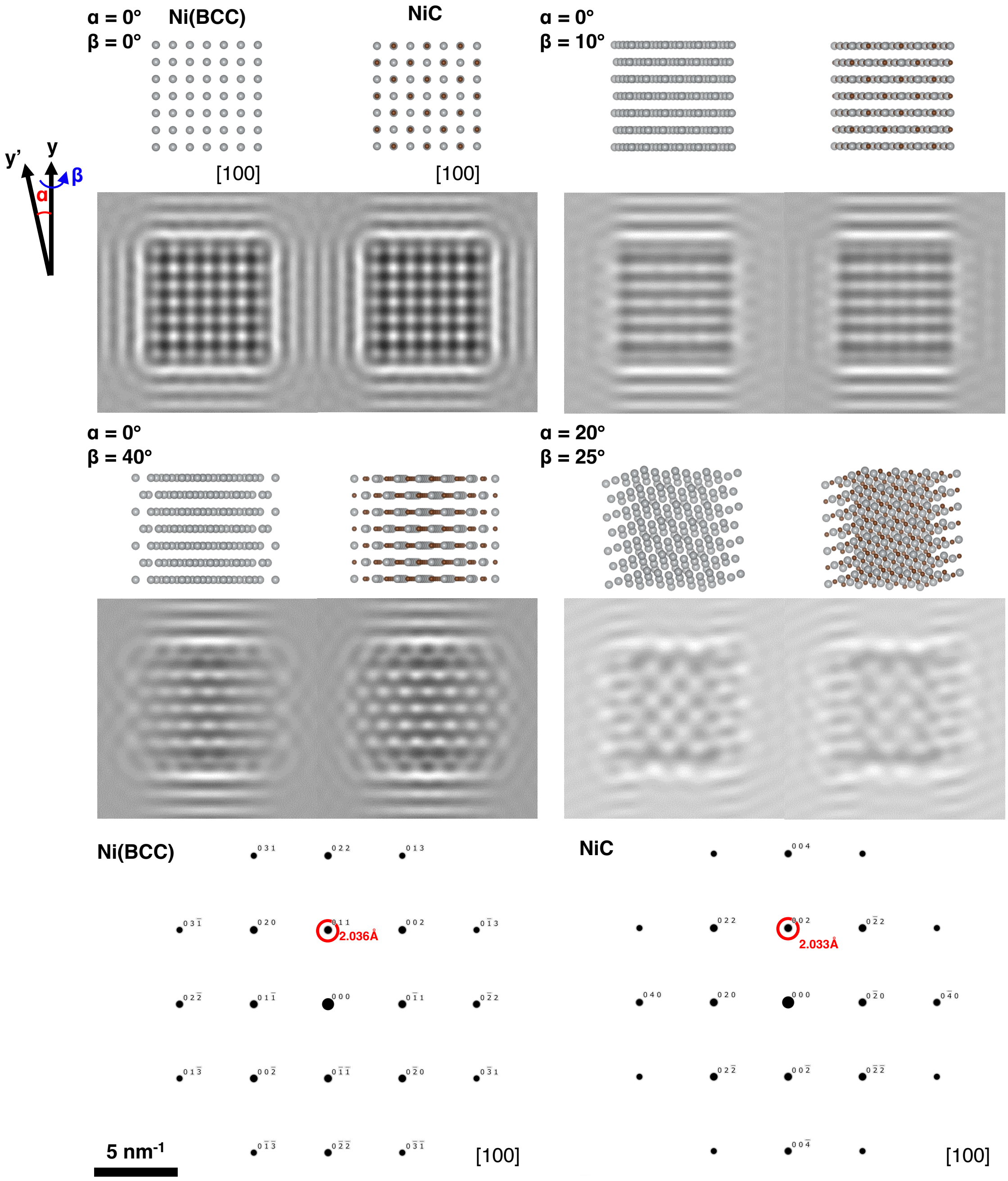


Figure S4. Simulated TEM images and diffraction patterns of Ni and NiC. The almost identical lattice constants do not allow for a differentiation between Ni and NiC under our experimental conditions.

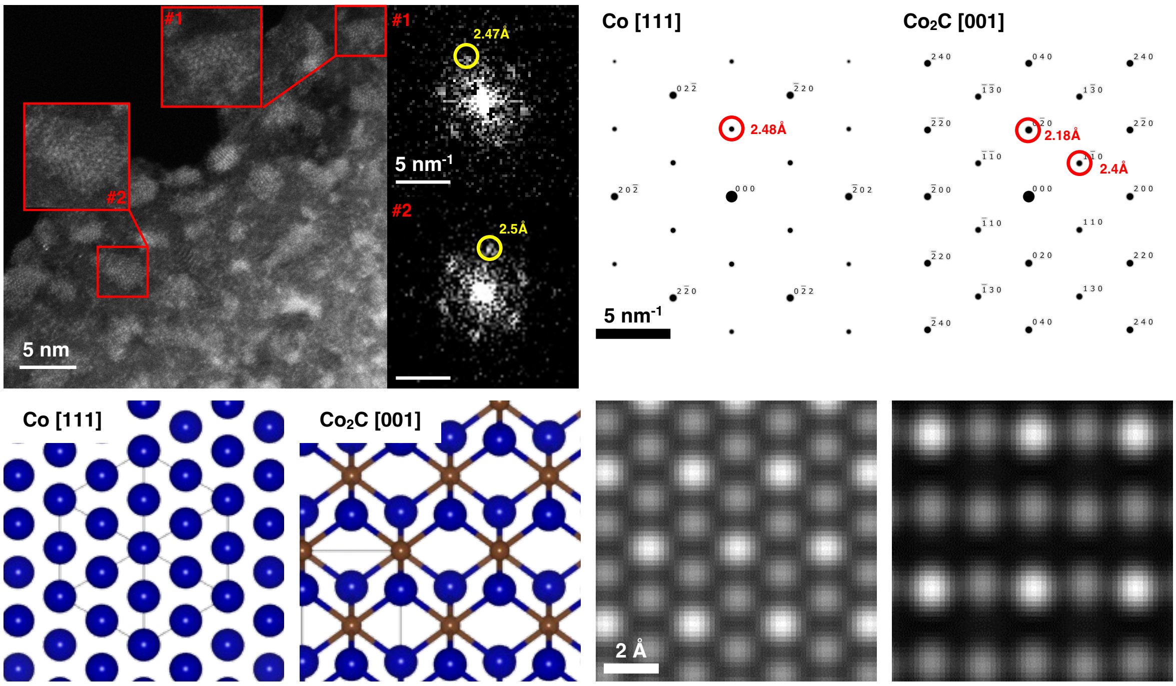


Figure S5. Simulated STEM images and diffraction patterns of Co and Co_2C in comparison with the experimental STEM images of Co clusters. Simulation reveals that the experimentally observed structures are metallic Co clusters.

2.4 Additional STEM-EDS Analysis

The omnipresent Au EDS signals stem from the gold grid.

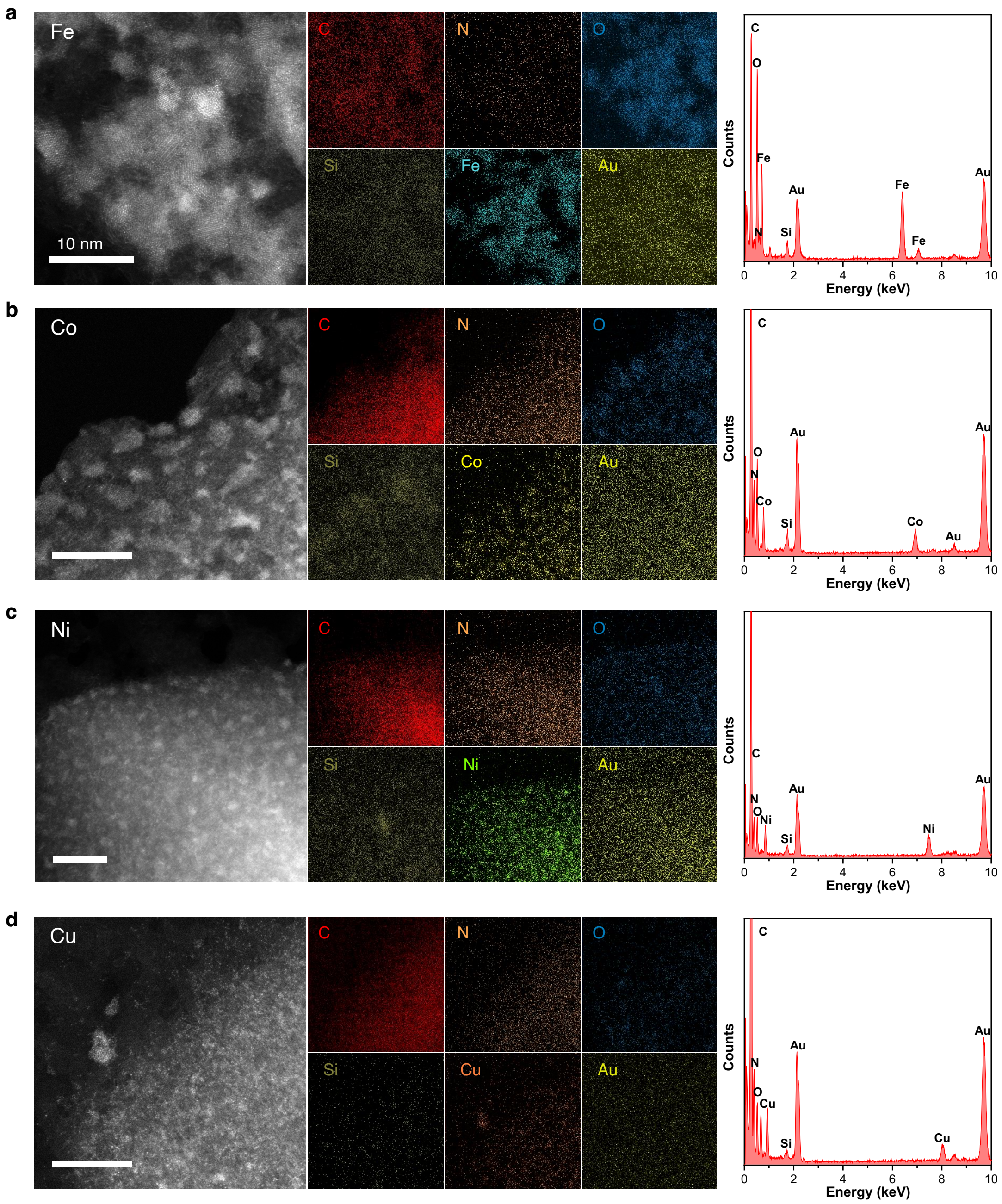


Figure S6. STEM-EDS analysis of **MTPP** samples after exposure to the e-beam in TEM mode. a) Fe. b) Co. c) Ni. d) Cu. 80 keV.

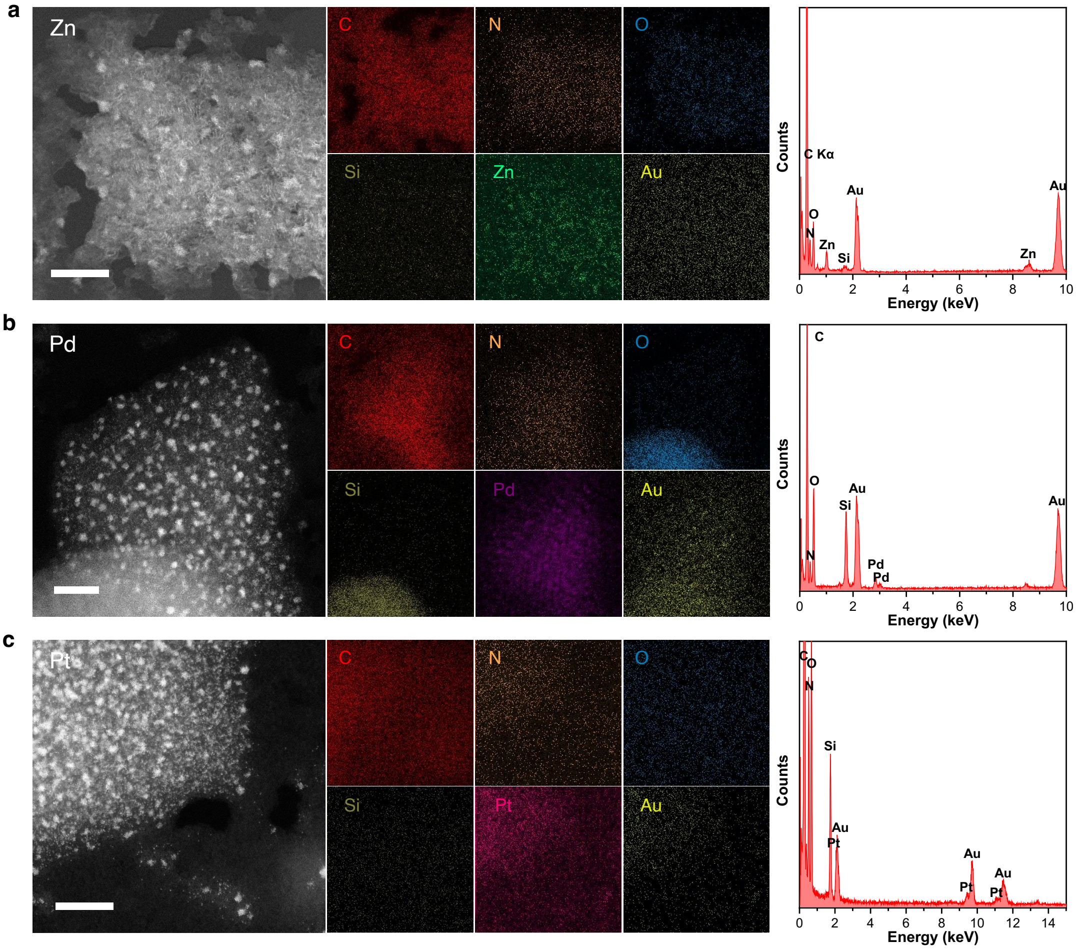


Figure S7. STEM-EDS analysis of **MTPP** samples after exposure to the e-beam in TEM mode. a) Zn. b) Pd. c) Pt. 80 keV.

3. Computational Section

3.1 Additional Mechanistic Explanations

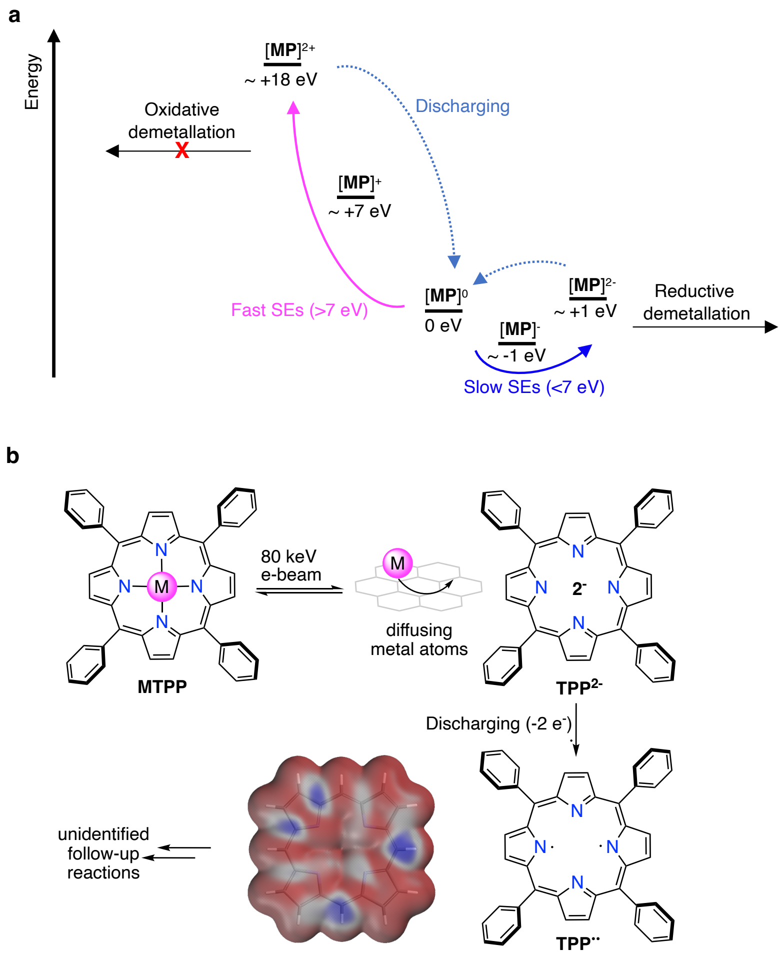


Figure S8. Proposed mechanistic pathways of **MTPPs** interacting with secondary electrons (SEs). a) SE-driven redox processes in metallo-porphyrins. Fast SEs can oxidize **MTPP** molecules, but will in the most cases not lead to the demetallation of the molecules. Electron attachment through slow SEs is likely to result in a reductive demetallation. b) Possible pathway for demetallated **TPP** molecules on the surface. Spin density map calculated at the ωB97X-D/6-311+G(2df,2p)//6-31G(d) level of theory; blue indicates a high spin density. Once **MTPP** gets demetallated, it is not in its equilibrium constitution. Therefore, the **TPP^{2-}** can either undergo a reversible recomplexation of a metal atom, or undergo further chemical events, such as the discharging to a neutral, open shell diradical, which will likely undergo further reactions due to its high reactivity.

3.2 Ionization of Metalloporphins

Table S1. Single point calculations of metalloporphins **MP**s at the density functional ωB97X-D/6-311+G(2df,2p)//6-31G(d) level of theory.

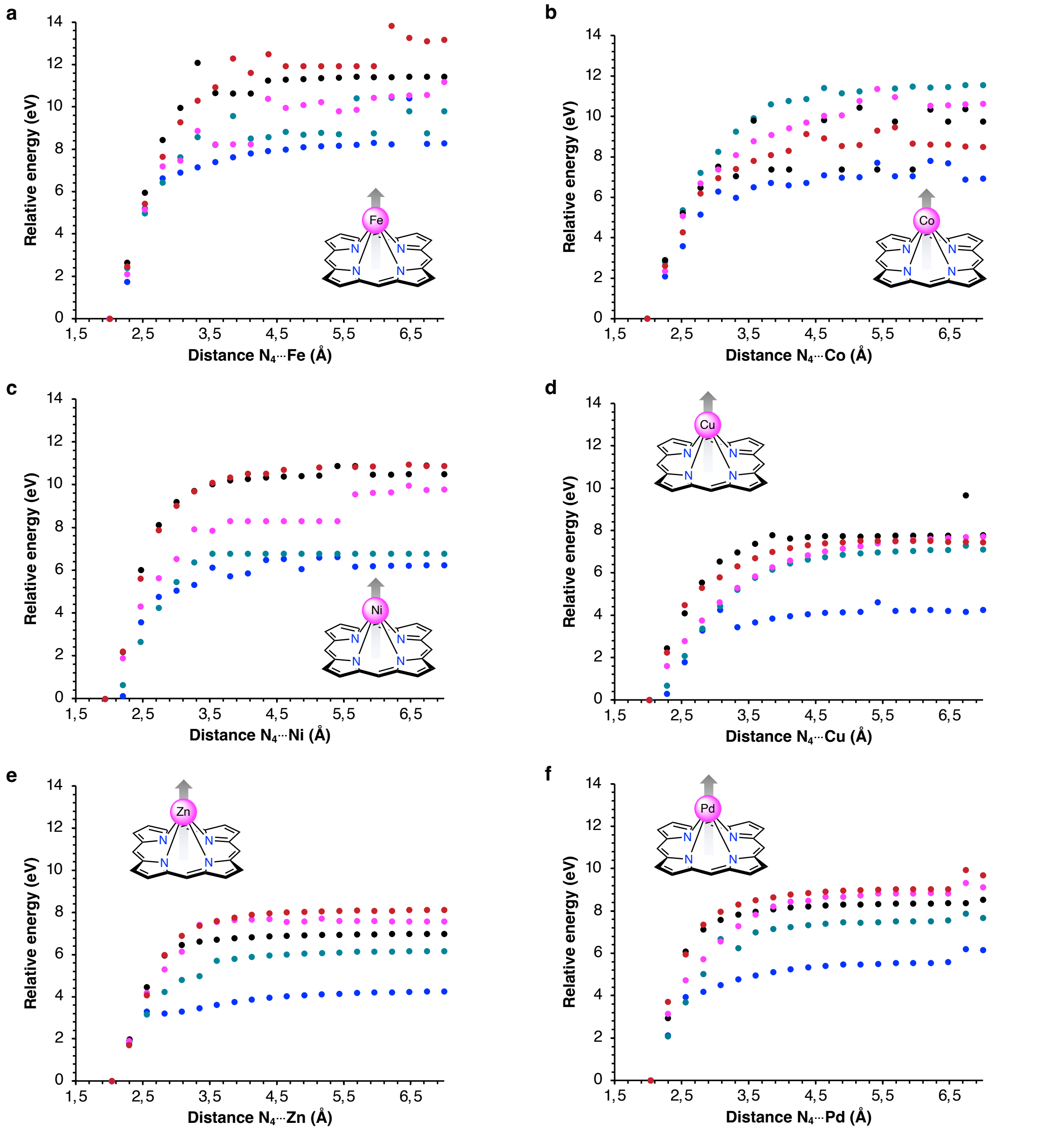
Entry	**MP**	**Charge**	***E* (hartree)**	**Δ*E* (hartree)**	**Δ*E* (eV)**
1	Fe	0	-2252,097296	0	0,0000
2		++	-2251,454647	0,642649	17,4874
3		+	-2251,804406	0,29289	7,9699
4		-	-2252,198957	-0,101661	-2,7663
5		--	-2252,058842	0,038454	1,0464
6	Co	0	-2371,21459	0	0,0000
7		++	-2370,573516	0,641074	17,4445
8		+	-2370,865037	0,349553	9,5118
9		-	-2371,248405	-0,033815	-0,9202
10		--	-2371,157894	0,056696	1,5428
11	Ni	0	-2496,774629	0	0,0000
12		++	-2496,109397	0,665232	18,1019
13		+	-2496,520989	0,25364	6,9019
14		-	-2496,803383	-0,028754	-0,7824
15		--	-2496,720897	0,053732	1,4621
16	Cu	0	-2628,942621	0	0,0000
17		++	-2628,269136	0,673485	18,3265
18		+	-2628,650909	0,291712	7,9379
19		-	-2628,967383	-0,024762	-0,6738
20		--	-2628,882042	0,060579	1,6484
21	Zn	0	-2767,831767	0	0,0000
22		++	-2767,185718	0,646049	17,5799
23		+	-2767,584456	0,247311	6,7297
24		-	-2767,878649	-0,046882	-1,2757
25		--	-2767,783337	0,04843	1,3178
26	Pd	0	-1116,347619	0	0,0000
27		++	-1115,693385	0,654234	17,8026
28		+	-1116,096461	0,251158	6,8344
29		-	-1116,394095	-0,046476	-1,2647
30		--	-1116,298581	0,049038	1,3344
31	Pt	0	-1107,833849	0	0,0000
32		++	-1107,176267	0,657582	17,8937
33		+	-1107,581216	0,252633	6,8745
34		-	-1107,877971	-0,044122	-1,2006
35		--	-1107,783264	0,050585	1,3765

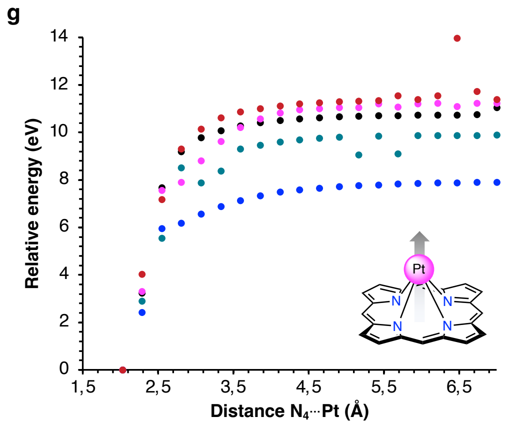
For comparative reasons, thermochemistry upon ionization was calculated at the density functional ωB97X-D/def2-TZVPPD//def2-SVP(D) level of theory.[1–4] The same trend in energetics is observed as for the cost-efficient ωB97X-D/6-311+G(2df,2p)//6-31G(d) calculations.

Table S2. Single point calculations of metalloporphins **MP**s at the density functional ωB97X-D/def2-TZVPPD//def2-SVP(D) level of theory.

Entry	**MP**	**Charge**	***E* (hartree)**	**Δ*E* (hartree)**	**Δ*E* (eV)**
36	Fe	0	-2252,052277	0	0,0000
37		++	-2251,400217	0,65206	17,7435
38		+	-2251,940622	0,111655	3,0383
39		-	-2252,257733	-0,205456	-5,5907
40		--	-2252,115662	-0,063385	-1,7248
41	Co	0	-2371,280172	0	0,0000
42		++	-2370,651791	0,628381	17,0991
43		+	-2370,943859	0,336313	9,1515
44		-	-2371,311364	-0,031192	-0,8488
45		--	-2371,22348	0,056692	1,5427
46	Ni	0	-2496,83693	0	0,0000
47		++	-2496,191296	0,645634	17,5686
48		+	-2496,590122	0,246808	6,7160
49		-	-2496,873972	-0,037042	-1,0080
50		--	-2496,783172	0,053758	1,4628
51	Cu	0	-2629,002978	0	0,0000
52		++	-2628,361189	0,641789	17,4640
53		+	-2628,64523	0,357748	9,7348
54		-	-2629,030112	-0,027134	-0,7384
55		--	-2628,944988	0,05799	1,5780
56	Zn	0	-2767,889791	0	0,0000
57		++	-2767,244932	0,644859	17,5475
58		+	-2767,640095	0,249696	6,7946
59		-	-2767,936544	-0,046753	-1,2722
60		--	-2767,842634	0,047157	1,2832
61	Pd	0	-1116,407825	0	0,0000
62		++	-1115,756079	0,651746	17,7349
63		+	-1116,157902	0,249923	6,8008
64		-	-1116,400788	0,007037	0,1915
65		--	-1116,3575	0,050325	1,3694
66	Pt	0	-1107,893223	0	0,0000
67		++	-1107,237843	0,65538	17,8338
68		+	-1107,635143	0,25808	7,0227
69		-	-1107,841049	0,052174	1,4197
70		--	-1107,841144	0,052079	1,4171

3.3 Morse Potentials of the Homolytic N_4-M Bond Cleavage





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	$E_d(N_4\cdots M)$ (eV)	$\Delta E_d(N_4\cdots M)$ (eV)			
M	$[MP]^0$	$[MP]^{2+}$	$[MP]^+$	$[MP]^-$	$[MP]^{2-}$
Fe	10.91	+0.11	-2.15	-2.82	-3.54
Co	9.50	-0.59	-0.22	+3.06	-2.82
Ni	10.23	+1.55	-3.01	-3.45	-3.90
Cu	7.24	+0.03	-0.72	-0.75	-3.21
Zn	6.80	+1.09	+0.89	-0.93	-3.01
Pd	8.08	+0.26	+0.15	-0.95	-3.22
Pt	10.38	+0.20	+0.42	-0.97	-2.96

Figure S9. Morse potentials for **MP**s in different ionization states, calculated at the density functional ωB97X-D/6-311G(2d,p)//6-31G(d) level of theory.

Table S3. Summary of Morse potential calculations for **FeP**.

Entry	Charge	M···N (Å)	*E* (hartree)	Δ*E* (hartree)	Δ*E* (eV)
71	++	2,003	-2251,43526	0	0,0000
72	++	2,266	-2251,34439	0,090866499	2,4726
73	++	2,529	-2251,23516	0,200093701	5,4448
74	++	2,792	-2251,15369	0,281562198	7,6617
75	++	3,055	-2251,09375	0,3415052	9,2928
76	++	3,318	-2251,05621	0,379049398	10,3145
77	++	3,581	-2251,03325	0,402011	10,9393
78	++	3,844	-2250,98355	0,451710898	12,2917
79	++	4,107	-2251,0079	0,427354101	11,6289
80	++	4,37	-2250,97571	0,459545199	12,5049
81	++	4,633	-2250,99686	0,4383929	11,9293
82	++	4,896	-2250,99683	0,438423	11,9301
83	++	5,159	-2250,99686	0,438392799	11,9293
84	++	5,422	-2250,99684	0,4384184	11,9300
85	++	5,685	-2250,99687	0,438386198	11,9291
86	++	5,948	-2250,99686	0,4383929	11,9293
87	++	6,211	-2250,92665	0,5086057	13,8399
88	++	6,474	-2250,94773	0,487528201	13,2663
89	++	6,737	-2250,95311	0,482146598	13,1199
90	++	7	-2250,95074	0,484519899	13,1845
91	+	2,002	-2251,83665	0	0,0000
92	+	2,265	-2251,75892	0,077732302	2,1152
93	+	2,528	-2251,64676	0,189886503	5,1671
94	+	2,791	-2251,57226	0,264395002	7,1946
95	+	3,054	-2251,56215	0,274497602	7,4695
96	+	3,317	-2251,51075	0,325895902	8,8681
97	+	3,58	-2251,53334	0,303307001	8,2534
98	+	3,843	-2251,53338	0,303266801	8,2523
99	+	4,106	-2251,53338	0,303266801	8,2523
100	+	4,369	-2251,45452	0,382128201	10,3982
101	+	4,633	-2251,47073	0,3659181	9,9571
102	+	4,896	-2251,46575	0,370904002	10,0928
103	+	5,159	-2251,4604	0,376255203	10,2384
104	+	5,422	-2251,47608	0,360574502	9,8117
105	+	5,685	-2251,4736	0,363055103	9,8792
106	+	5,948	-2251,4526	0,3840512	10,4506
107	+	6,211	-2251,45066	0,385987002	10,5032
108	+	6,474	-2251,44902	0,387628902	10,5479
109	+	6,737	-2251,44793	0,3887158	10,5775
110	+	7	-2251,42575	0,4109024	11,1812
111	0	2,002	-2252,05052	0	0,0000
112	0	2,265	-2251,95335	0,097168598	2,6441

113	0	2,528	-2251,8318	0,2187167	5,9516
114	0	2,791	-2251,74022	0,310292099	8,4435
115	0	3,054	-2251,68441	0,366109498	9,9624
116	0	3,317	-2251,60586	0,4446528	12,0996
117	0	3,58	-2251,65866	0,391855199	10,6629
118	0	3,843	-2251,6596	0,390916299	10,6374
119	0	4,106	-2251,6596	0,390916198	10,6374
120	0	4,369	-2251,63706	0,413456898	11,2507
121	0	4,633	-2251,6352	0,415316898	11,3014
122	0	4,896	-2251,63413	0,416387498	11,3305
123	0	5,159	-2251,63295	0,417568799	11,3626
124	0	5,422	-2251,63215	0,418362301	11,3842
125	0	5,685	-2251,63044	0,420079801	11,4310
126	0	5,948	-2251,63109	0,419420898	11,4130
127	0	6,211	-2251,63073	0,419786599	11,4230
128	0	6,474	-2251,6305	0,420016598	11,4292
129	0	6,737	-2251,63016	0,4203557	11,4385
130	0	7	-2251,63002	0,420492198	11,4422
131	-	2,003	-2252,14717	0	0,0000
132	-	2,266	-2252,0585	0,0886769	2,4130
133	-	2,529	-2251,96357	0,1836023	4,9961
134	-	2,792	-2251,91078	0,236395698	6,4327
135	-	3,055	-2251,86626	0,2809132	7,6440
136	-	3,318	-2251,83163	0,3155379	8,5862
137	-	3,581	-2251,84497	0,302202199	8,2233
138	-	3,844	-2251,79503	0,3521397	9,5822
139	-	4,107	-2251,83435	0,312826	8,5124
140	-	4,37	-2251,8319	0,315276399	8,5791
141	-	4,633	-2251,8228	0,324373897	8,8267
142	-	4,896	-2251,82792	0,319250397	8,6873
143	-	5,159	-2251,82409	0,3230801	8,7915
144	-	5,422	-2251,82662	0,3205535	8,7227
145	-	5,685	-2251,76425	0,382920198	10,4198
146	-	5,948	-2251,82526	0,321917098	8,7598
147	-	6,211	-2251,76373	0,383445498	10,4341
148	-	6,474	-2251,78708	0,360092599	9,7986
149	-	6,737	-2251,82478	0,3223885	8,7726
150	-	7	-2251,78701	0,360159397	9,8004
151	--	2,002	-2251,99285	0	0,0000
152	--	2,265	-2251,92846	0,064394902	1,7523
153	--	2,528	-2251,80139	0,191463701	5,2100
154	--	2,791	-2251,74854	0,2443133	6,6481
155	--	3,054	-2251,73893	0,253929202	6,9098
156	--	3,317	-2251,72939	0,2634665	7,1693
157	--	3,58	-2251,72032	0,2725338	7,4160

158	--	3,843	-2251,71241	0,280440003	7,6312
159	--	4,106	-2251,70587	0,2869795	7,8091
160	--	4,369	-2251,70189	0,2909685	7,9177
161	--	4,633	-2251,69866	0,2941918	8,0054
162	--	4,896	-2251,69519	0,297667902	8,1000
163	--	5,159	-2251,69332	0,299533103	8,1507
164	--	5,422	-2251,69193	0,300924901	8,1886
165	--	5,685	-2251,69085	0,302005	8,2180
166	--	5,948	-2251,68751	0,305344403	8,3088
167	--	6,211	-2251,69007	0,3027841	8,2392
168	--	6,474	-2251,60967	0,3831845	10,4270
169	--	6,737	-2251,68912	0,303738203	8,2651
170	--	7	-2251,68833	0,304527201	8,2866

Table S4. Summary of Morse potential calculations for **CoP**.

Entry	Charge	M···N (Å)	*E* (hartree)	Δ*E* (hartree)	Δ*E* (eV)
171	++	1,985	-2370,54585	0	0
172	++	2,249	-2370,44979	0,096057598	2,613861709
173	++	2,513	-2370,38901	0,1568438	4,267939379
174	++	2,777	-2370,31884	0,227005698	6,177142851
175	++	3,041	-2370,29069	0,2551631	6,943345179
176	++	3,305	-2370,27377	0,272080798	7,403699427
177	++	3,569	-2370,25943	0,286418397	7,793845568
178	++	3,833	-2370,24836	0,2974898	8,095113944
179	++	4,097	-2370,24132	0,3045271	8,286608729
180	++	4,361	-2370,21029	0,3355552	9,130926769
181	++	4,624	-2370,21785	0,327999797	8,925333676
182	++	4,888	-2370,23198	0,313872598	8,540912813
183	++	5,152	-2370,23084	0,315008	8,571808691
184	++	5,416	-2370,20394	0,3419098	9,303844332
185	++	5,68	-2370,19789	0,347954597	9,468331721
186	++	5,944	-2370,22812	0,317728698	8,645842693
187	++	6,208	-2370,22922	0,316628799	8,615912901
188	++	6,472	-2370,22961	0,316243198	8,605420158
189	++	6,736	-2370,23298	0,312872499	8,513698719
190	++	7	-2370,23393	0,3119209	8,487804378
191	+	1,988	-2370,86017	0	0
192	+	2,252	-2370,77362	0,086550903	2,355171231
193	+	2,516	-2370,6733	0,186874203	5,085108688
194	+	2,779	-2370,61424	0,245932903	6,692178597
195	+	3,043	-2370,58923	0,270942602	7,37272752
196	+	3,307	-2370,56295	0,297226202	8,087941073
197	+	3,571	-2370,53792	0,322248701	8,768838302

198	+	3,835	-2370,52633	0,333837502	9,084185802
199	+	4,098	-2370,51397	0,3462031	9,420671035
200	+	4,362	-2370,50411	0,3560648	9,689021699
201	+	4,626	-2370,4918	0,368374702	10,02399137
202	+	4,89	-2370,49057	0,369601503	10,05737434
203	+	5,153	-2370,46433	0,395838503	10,77131984
204	+	5,417	-2370,44279	0,4173811	11,35752406
205	+	5,681	-2370,45791	0,402264003	10,94616669
206	+	5,945	-2369,83427	1,0259014	27,91621336
207	+	6,209	-2370,47379	0,3863835	10,51403597
208	+	6,472	-2370,47283	0,3873385	10,54002286
209	+	6,736	-2370,47097	0,389198601	10,59063881
210	+	7	-2370,47021	0,3899584	10,61131401
211	0	1,988	-2371,17306	0	0
212	0	2,252	-2371,06625	0,106801603	2,90622114
213	0	2,516	-2370,9811	0,191951901	5,223279959
214	0	2,779	-2370,93501	0,238047302	6,477600354
215	0	3,043	-2370,89665	0,276409	7,521475863
216	0	3,307	-2370,91398	0,2590736	7,049755359
217	0	3,571	-2370,81283	0,360221002	9,802117774
218	0	3,835	-2370,90244	0,270616502	7,363853883
219	0	4,098	-2370,90245	0,270606	7,363568108
220	0	4,362	-2370,65242	0,520631902	14,16712294
221	0	4,626	-2370,81243	0,360628702	9,813211862
222	0	4,89	-2370,90244	0,270615101	7,363815759
223	0	5,153	-2370,78943	0,3836293	10,43909033
224	0	5,417	-2370,90244	0,2706163	7,363848386
225	0	5,681	-2370,81501	0,3580405	9,742783262
226	0	5,945	-2370,90244	0,270619202	7,363927353
227	0	6,209	-2370,79288	0,380177602	10,3451648
228	0	6,472	-2370,81492	0,3581382	9,745441815
229	0	6,736	-2370,79264	0,380417001	10,35167918
230	0	7	-2370,81471	0,358348101	9,751153516
231	-	1,985	-2371,19953	0	0
232	-	2,249	-2371,09671	0,102819201	2,797854406
233	-	2,513	-2371,0026	0,196928199	5,358691994
234	-	2,777	-2370,93453	0,264996	7,210912154
235	-	3,041	-2370,89596	0,303569	8,260537487
236	-	3,305	-2370,85961	0,339911498	9,249467737
237	-	3,569	-2370,83516	0,3643656	9,914898088
238	-	3,833	-2370,8104	0,389129497	10,58875839
239	-	4,097	-2370,80384	0,395690598	10,76729514
240	-	4,361	-2370,80067	0,398854099	10,85337843
241	-	4,624	-2370,78032	0,419209998	11,40729094
242	-	4,888	-2370,79007	0,409456197	11,14187636

243	-	5,152	-2370,78676	0,412761997	11,23183181
244	-	5,416	-2370,20394	0,9955866	27,09130521
245	-	5,68	-2370,78163	0,4178936	11,37146991
246	-	5,944	-2370,7779	0,421627399	11,47307181
247	-	6,208	-2370,77978	0,419748098	11,42193339
248	-	6,472	-2370,77835	0,4211758	11,46078316
249	-	6,736	-2370,7753	0,4242214	11,5436582
250	-	7	-2370,77499	0,424538501	11,55228697
251	--	1,985	-2371,12735	0	0
252	--	2,249	-2371,05099	0,076361202	2,077895204
253	--	2,513	-2370,99559	0,131761	3,585401275
254	--	2,777	-2370,93824	0,189107999	5,145893404
255	--	3,041	-2370,89626	0,2310936	6,288380387
256	--	3,305	-2370,9077	0,219652001	5,97703846
257	--	3,569	-2370,88875	0,2385979	6,492582896
258	--	3,833	-2370,88105	0,246300902	6,702192365
259	--	4,097	-2370,88507	0,242278103	6,592726372
260	--	4,361	-2370,88117	0,246182401	6,698967787
261	--	4,624	-2370,86681	0,260539602	7,089647326
262	--	4,888	-2370,87144	0,255913001	6,963751035
263	--	5,152	-2370,87032	0,257025402	6,994021024
264	--	5,416	-2370,84413	0,283215001	7,706676678
265	--	5,68	-2370,86817	0,259175099	7,052517289
266	--	5,944	-2370,86835	0,259000201	7,047758069
267	--	6,208	-2370,84074	0,286607001	7,798977747
268	--	6,472	-2370,84508	0,282272801	7,681038097
269	--	6,736	-2370,8745	0,252844103	6,880242024
270	--	7	-2370,87327	0,254080202	6,913878009

Table S5. Summary of Morse potential calculations for **NiP**.

Entry	**Charge**	**M···N (Å)**	***E* (hartree)**	**Δ*E* (hartree)**	**Δ*E* (eV)**
271	++	1,934	-2496,10848	0	0
272	++	2,201	-2496,02751	0,080969103	2,203282641
273	++	2,467	-2495,90241	0,2060696	5,607442313
274	++	2,734	-2495,81898	0,289498102	7,877648653
275	++	3,001	-2495,7767	0,3317779	9,028141148
276	++	3,267	-2495,75181	0,356669001	9,705462854
277	++	3,534	-2495,73762	0,370859902	10,09161714
278	++	3,8	-2495,72869	0,3797937	10,33471829
279	++	4,067	-2495,72211	0,386375602	10,51382106
280	++	4,334	-2495,72211	0,3863714	10,51370671
281	++	4,6	-2495,71507	0,393415403	10,7053839
282	++	4,867	-2495,54222	0,566263299	15,40881713

283	++	5,134	-2495,71091	0,3975753	10,81858052
284	++	5,4	-2495,54338	0,565100003	15,37716222
285	++	5,667	-2495,70983	0,398653403	10,84791721
286	++	5,933	-2495,70913	0,3993534	10,86696511
287	++	6,2	-2495,54333	0,5651531	15,37860707
288	++	6,467	-2495,70611	0,4023748	10,94918163
289	++	6,733	-2495,70873	0,399748601	10,87771908
290	++	7	-2495,70872	0,399763603	10,87812731
291	+	1,934	-2496,48554	0	0
292	+	2,201	-2496,41617	0,069369897	1,887652021
293	+	2,467	-2496,32655	0,158985298	4,326212538
294	+	2,734	-2496,27868	0,206862301	5,629012817
295	+	3,001	-2496,24529	0,240247399	6,537468073
296	+	3,267	-2496,19424	0,2912976	7,926615513
297	+	3,534	-2496,19682	0,2887243	7,856592417
298	+	3,8	-2496,17995	0,3055939	8,31563785
299	+	4,067	-2496,17995	0,305594299	8,315648708
300	+	4,334	-2496,17995	0,305594098	8,315643238
301	+	4,6	-2496,17995	0,305594098	8,315643238
302	+	4,867	-2496,17995	0,305594098	8,315643238
303	+	5,134	-2496,17995	0,305594198	8,315645959
304	+	5,4	-2496,17995	0,305594098	8,315643238
305	+	5,667	-2496,13451	0,351031698	9,552063947
306	+	5,933	-2496,13137	0,354165599	9,637341781
307	+	6,2	-2496,13058	0,354961298	9,658993864
308	+	6,467	-2496,11972	0,3658204	9,954485233
309	+	6,733	-2496,12683	0,3587097	9,760993131
310	+	7	-2496,12614	0,359397497	9,77970905
311	0	1,935	-2496,7273	0	0
312	0	2,202	-2496,6467	0,080593597	2,193064608
313	0	2,468	-2496,50622	0,221075598	6,015776527
314	0	2,735	-2496,42903	0,298267398	8,116273474
315	0	3,001	-2496,38918	0,3381234	9,200811087
316	0	3,268	-2496,36998	0,357322898	9,723256307
317	0	3,534	-2496,35876	0,368539497	10,02847567
318	0	3,801	-2496,35231	0,374990299	10,20401102
319	0	4,068	-2496,34946	0,377840698	10,28157437
320	0	4,334	-2496,34751	0,379786897	10,33453317
321	0	4,601	-2496,34589	0,381412998	10,37878165
322	0	4,867	-2496,34451	0,382787697	10,41618914
323	0	5,134	-2496,34384	0,383455597	10,43436363
324	0	5,401	-2496,32772	0,399580199	10,87313663
325	0	5,667	-2496,32709	0,400210399	10,89028525
326	0	5,934	-2496,34223	0,385066196	10,47819029
327	0	6,2	-2496,34182	0,385476798	10,48936334

328	0	6,467	-2496,3414	0,3858977	10,50081667
329	0	6,733	-2496,32643	0,400869098	10,90820937
330	0	7	-2496,34107	0,386231098	10,5098889
331	-	1,933	-2496,75315	0	0
332	-	2,2	-2496,72941	0,023742002	0,6460531
333	-	2,466	-2496,65552	0,0976284	2,656605436
334	-	2,733	-2496,5969	0,156249799	4,251775781
335	-	3	-2496,55266	0,200493999	5,455722404
336	-	3,266	-2496,51911	0,234039899	6,368553308
337	-	3,533	-2496,50382	0,249327701	6,784555803
338	-	3,8	-2496,50382	0,2493289	6,784588429
339	-	4,066	-2496,50382	0,249329001	6,784591178
340	-	4,333	-2496,50382	0,249332998	6,784699942
341	-	4,6	-2496,50382	0,249327101	6,784539476
342	-	4,867	-2496,50382	0,2493295	6,784604756
343	-	5,133	-2496,50382	0,249327701	6,784555803
344	-	5,4	-2496,50382	0,249327399	6,784547585
345	-	5,667	-2496,50382	0,249327701	6,784555803
346	-	5,933	-2496,50382	0,249327701	6,784555803
347	-	6,2	-2496,50382	0,249328401	6,784574851
348	-	6,467	-2496,50382	0,249327701	6,784555803
349	-	6,733	-2496,50382	0,249327999	6,784563912
350	-	7	-2496,50382	0,2493295	6,784604756
351	--	1,935	-2496,62854	0	0
352	--	2,202	-2496,62364	0,0048967	0,133246073
353	--	2,468	-2496,49734	0,131202001	3,57019013
354	--	2,735	-2496,45325	0,175292302	4,769948947
355	--	3,001	-2496,44236	0,186174002	5,066055238
356	--	3,268	-2496,43304	0,195493501	5,319651853
357	--	3,534	-2496,40345	0,225088302	6,124967821
358	--	3,801	-2496,41828	0,210255001	5,721332934
359	--	4,068	-2496,41279	0,215750702	5,870878652
360	--	4,334	-2496,39038	0,2381563	6,480566342
361	--	4,601	-2496,38845	0,240084	6,533021758
362	--	4,867	-2496,4054	0,223136	6,07184295
363	--	5,134	-2496,3861	0,2424368	6,59704474
364	--	5,401	-2496,38508	0,243460502	6,624901104
365	--	5,667	-2496,40177	0,2267703	6,170737341
366	--	5,934	-2496,40091	0,2276306	6,194147309
367	--	6,2	-2496,4	0,228533901	6,218727394
368	--	6,467	-2496,39996	0,228574801	6,21984034
369	--	6,733	-2496,39948	0,229061801	6,233092292
370	--	7	-2496,39922	0,229318701	6,2400829

Table S6. Summary of Morse potential calculations for **CuP**.

Entry	Charge	M···N (Å)	*E* (hartree)	Δ*E* (hartree)	Δ*E* (eV)
371	++	2,016	-2628,27881	0	0
372	++	2,278	-2628,19614	0,082672298	2,24962897
373	++	2,541	-2628,11369	0,165125299	4,493290561
374	++	2,803	-2628,08388	0,194931798	5,304367128
375	++	3,065	-2628,06575	0,2130582	5,797611903
376	++	3,328	-2628,04587	0,232942499	6,338691517
377	++	3,59	-2628,03177	0,247046798	6,722489239
378	++	3,852	-2628,02098	0,257832401	7,015980597
379	++	4,115	-2628,01446	0,2643549	7,193466926
380	++	4,377	-2628,00961	0,269205	7,325444937
381	++	4,639	-2628,00667	0,272141401	7,405348519
382	++	4,901	-2628,00481	0,2740006	7,455939927
383	++	5,164	-2628,00245	0,2763572	7,520066312
384	++	5,426	-2628,00191	0,276906598	7,535016201
385	++	5,688	-2628,00229	0,2765196	7,524485443
386	++	5,951	-2628,00176	0,277047399	7,538847593
387	++	6,213	-2628,00203	0,276786298	7,531742669
388	++	6,475	-2628,00373	0,275083598	7,485409819
389	++	6,738	-2628,00393	0,274881199	7,479902258
390	++	7	-2628,00506	0,273750201	7,449126219
391	+	2,016	-2628,61973	0	0
392	+	2,278	-2628,56055	0,059175499	1,610248168
393	+	2,541	-2628,51682	0,102906898	2,800240764
394	+	2,803	-2628,48101	0,1387171	3,774686495
395	+	3,065	-2628,44966	0,170064099	4,627682224
396	+	3,328	-2628,42444	0,195287298	5,314040781
397	+	3,59	-2628,40463	0,215095799	5,853057825
398	+	3,852	-2628,38906	0,2306647	6,276709418
399	+	4,115	-2628,37722	0,2425065	6,598941374
400	+	4,377	-2628,36832	0,251403298	6,841035703
401	+	4,639	-2628,36139	0,258334197	7,029635168
402	+	4,901	-2628,35619	0,263537899	7,171235185
403	+	5,164	-2628,35198	0,2677413	7,285615611
404	+	5,426	-2628,34722	0,2725062	7,415275211
405	+	5,688	-2628,34431	0,275416598	7,494471215
406	+	5,951	-2628,34177	0,277953599	7,563506564
407	+	6,213	-2628,33972	0,280001499	7,61923279
408	+	6,475	-2628,33802	0,281707399	7,665652717
409	+	6,738	-2628,3367	0,283020597	7,701386673
410	+	7	-2628,33537	0,284352299	7,737624149
411	0	2,016	-2628,89552	0	0
412	0	2,278	-2628,80532	0,090200502	2,454481951

413	0	2,541	-2628,74483	0,1506938	4,100589269
414	0	2,803	-2628,69132	0,2042045	5,556690331
415	0	3,065	-2628,65493	0,240589902	6,546788059
416	0	3,328	-2628,63878	0,2567432	6,986341912
417	0	3,59	-2628,62371	0,271809801	7,396325219
418	0	3,852	-2628,60855	0,286970399	7,808866315
419	0	4,115	-2628,61433	0,281190801	7,651595362
420	0	4,377	-2628,6119	0,2836251	7,717836046
421	0	4,639	-2628,61093	0,284590703	7,744111456
422	0	4,901	-2628,61051	0,285011102	7,755551101
423	0	5,164	-2628,61104	0,284486502	7,741276001
424	0	5,426	-2628,61063	0,284894101	7,75236734
425	0	5,688	-2628,61011	0,285406999	7,766324013
426	0	5,951	-2628,60996	0,285559401	7,770471084
427	0	6,213	-2628,61005	0,285467699	7,767975745
428	0	6,475	-2628,60963	0,285892099	7,779524263
429	0	6,738	-2628,53996	0,355560903	9,675309956
430	0	7	-2628,60929	0,2862317	7,788765281
431	-	2,019	-2628,92142	0	0
432	-	2,281	-2628,89578	0,025632002	0,697482646
433	-	2,543	-2628,84405	0,077363301	2,105163732
434	-	2,805	-2628,79672	0,1246964	3,393163619
435	-	3,068	-2628,75821	0,163204599	4,441025625
436	-	3,33	-2628,72952	0,191897999	5,22181321
437	-	3,592	-2628,70902	0,2123936	5,779527207
438	-	3,854	-2628,69451	0,226909298	6,174519672
439	-	4,116	-2628,68393	0,237484898	6,462296553
440	-	4,378	-2628,67752	0,243896998	6,636778771
441	-	4,641	-2628,67267	0,2487492	6,768813981
442	-	4,903	-2628,66861	0,252805401	6,879188889
443	-	5,165	-2628,66619	0,255224299	6,94501049
444	-	5,427	-2628,66447	0,256943401	6,991789662
445	-	5,689	-2628,66305	0,258368	7,030554995
446	-	5,951	-2628,66219	0,259225801	7,053896961
447	-	6,214	-2628,66096	0,2604586	7,087443148
448	-	6,476	-2628,66078	0,260637999	7,092324846
449	-	6,738	-2628,6528	0,268610999	7,309281338
450	-	7	-2628,6598	0,2616117	7,118820613
451	--	2,019	-2628,82331	0	0
452	--	2,281	-2628,8121	0,011206701	0,304950034
453	--	2,543	-2628,75683	0,066477299	1,808940366
454	--	2,805	-2628,70218	0,121131398	3,296154924
455	--	3,068	-2628,66657	0,156733599	4,264940656
456	--	3,33	-2628,69655	0,126755901	3,449205524
457	--	3,592	-2628,68824	0,135069799	3,675438329

458	--	3,854	-2628,6817	0,141608201	3,853357401
459	--	4,116	-2628,67722	0,146089401	3,975297126
460	--	4,378	-2628,67413	0,149181999	4,059451048
461	--	4,641	-2628,67165	0,1516615	4,126921741
462	--	4,903	-2628,67056	0,1527525	4,156609379
463	--	5,165	-2628,6695	0,153809398	4,185369053
464	--	5,427	-2628,6532	0,170104899	4,628792449
465	--	5,689	-2628,66782	0,155492399	4,231165866
466	--	5,951	-2628,66698	0,1563242	4,253800336
467	--	6,214	-2628,66675	0,1565548	4,260075285
468	--	6,476	-2628,6684	0,154908199	4,215268966
469	--	6,738	-2628,66986	0,153444301	4,175434252
470	--	7	-2628,66607	0,157240301	4,278728727

Table S7. Summary of Morse potential calculations for **ZnP**.

Entry	Charge	M···N (Å)	*E* (hartree)	Δ*E* (hartree)	Δ*E* (eV)
471	++	2,034	-2767,16985	0	0
472	++	2,295	-2767,1072	0,0626528	1,704870407
473	++	2,557	-2767,01978	0,150067702	4,083552266
474	++	2,818	-2766,94968	0,220170602	5,991150319
475	++	3,079	-2766,91593	0,253918502	6,909477925
476	++	3,341	-2766,89894	0,270909101	7,371815911
477	++	3,602	-2766,8901	0,279750701	7,612408225
478	++	3,864	-2766,88418	0,285672899	7,773559524
479	++	4,125	-2766,87972	0,2901343	7,894960491
480	++	4,386	-2766,87674	0,293106601	7,975840962
481	++	4,648	-2766,875	0,294845	8,023145233
482	++	4,909	-2766,87429	0,295558799	8,042568703
483	++	5,17	-2766,87339	0,2964563	8,066990962
484	++	5,432	-2766,87302	0,2968303	8,077168025
485	++	5,693	-2766,87146	0,298389602	8,119598816
486	++	5,955	-2766,87256	0,297293801	8,089780537
487	++	6,216	-2766,87243	0,297420301	8,093222779
488	++	6,477	-2766,87115	0,2986991	8,12802069
489	++	6,739	-2766,87098	0,298873499	8,132766331
490	++	7	-2766,87089	0,298961699	8,135166376
491	+	2,034	-2767,54397	0	0
492	+	2,295	-2767,47361	0,0703649	1,914727437
493	+	2,557	-2767,38943	0,1545408	4,205271525
494	+	2,818	-2767,34911	0,1948626	5,302484154
495	+	3,079	-2767,31815	0,225818001	6,144823952
496	+	3,341	-2767,27077	0,273199301	7,434135459
497	+	3,602	-2767,26569	0,278284103	7,57250004

498	+	3,864	-2767,26305	0,2809247	7,644354382
499	+	4,125	-2767,26199	0,2819851	7,67320935
500	+	4,386	-2767,26127	0,282703303	7,692752659
501	+	4,648	-2767,26595	0,278017402	7,565242733
502	+	4,909	-2767,26516	0,278808501	7,586769644
503	+	5,17	-2767,26015	0,283823401	7,723232094
504	+	5,432	-2767,2645	0,279473603	7,604868001
505	+	5,693	-2767,26405	0,2799192	7,616993319
506	+	5,955	-2767,26419	0,279779103	7,613181083
507	+	6,216	-2767,26542	0,278548103	7,57968385
508	+	6,477	-2767,26519	0,2787796	7,585983207
509	+	6,739	-2767,26503	0,278944701	7,590475837
510	+	7	-2767,26509	0,278880302	7,58872345
511	0	2,035	-2767,78629	0	0
512	0	2,296	-2767,71335	0,0729439	1,984905635
513	0	2,558	-2767,62186	0,1644256	4,474250772
514	0	2,819	-2767,56717	0,2191227	5,962635439
515	0	3,08	-2767,54889	0,2374001	6,459989081
516	0	3,342	-2767,54232	0,243970398	6,638776088
517	0	3,603	-2767,53951	0,246776398	6,715131277
518	0	3,864	-2767,53703	0,249261297	6,782748857
519	0	4,126	-2767,53547	0,250820599	6,825179648
520	0	4,387	-2767,5337	0,252593998	6,873436317
521	0	4,648	-2767,53258	0,253706399	6,903706306
522	0	4,909	-2767,53203	0,254256297	6,9186698
523	0	5,171	-2767,53117	0,2551209	6,942196858
524	0	5,432	-2767,53058	0,255712397	6,95829232
525	0	5,693	-2767,53034	0,255952697	6,964831219
526	0	5,955	-2767,52984	0,256446	6,978254684
527	0	6,216	-2767,52961	0,256683398	6,984714616
528	0	6,477	-2767,52949	0,256800599	6,98790382
529	0	6,739	-2767,52919	0,257099699	6,996042749
530	0	7	-2767,52909	0,2572027	6,998845551
531	-	2,035	-2767,8312	0	0
532	-	2,296	-2767,76024	0,070955701	1,930803968
533	-	2,558	-2767,7147	0,116495799	3,170013785
534	-	2,819	-2767,67523	0,155969702	4,244153949
535	-	3,08	-2767,65477	0,176424902	4,800768578
536	-	3,342	-2767,64799	0,1832138	4,985503997
537	-	3,603	-2767,6209	0,210295502	5,722435023
538	-	3,864	-2767,61741	0,2137926	5,817595956
539	-	4,126	-2767,6141	0,217098001	5,907540544
540	-	4,387	-2767,61215	0,219051402	5,96069532
541	-	4,648	-2767,60974	0,221462201	6,026296536
542	-	4,909	-2767,60861	0,222591501	6,05702637

543	-	5,171	-2767,60785	0,2233475	6,077598162
544	-	5,432	-2767,60662	0,224576	6,111027366
545	-	5,693	-2767,60546	0,2257412	6,14273409
546	-	5,955	-2767,60519	0,226012301	6,150111127
547	-	6,216	-2767,60512	0,226082899	6,152032198
548	-	6,477	-2767,60459	0,2266117	6,166421613
549	-	6,739	-2767,60439	0,226809401	6,171801334
550	-	7	-2767,60413	0,2270675	6,17882457
551	--	2,034	-2767,74379	0	0
552	--	2,295	-2767,67818	0,065604802	1,785198515
553	--	2,557	-2767,62215	0,121641301	3,310030098
554	--	2,818	-2767,62584	0,117947299	3,209511132
555	--	3,079	-2767,62193	0,121860299	3,31598934
556	--	3,341	-2767,61632	0,127467699	3,468574545
557	--	3,602	-2767,61063	0,1331545	3,623320361
558	--	3,864	-2767,60588	0,137903299	3,75254183
559	--	4,125	-2767,60154	0,1422516	3,870865188
560	--	4,386	-2767,59813	0,145658001	3,963558128
561	--	4,648	-2767,59578	0,148009602	4,027548484
562	--	4,909	-2767,59387	0,149920002	4,079533142
563	--	5,17	-2767,59221	0,151581202	4,12473672
564	--	5,432	-2767,59093	0,152860001	4,159534631
565	--	5,693	-2767,58988	0,153904703	4,187962435
566	--	5,955	-2767,58914	0,154647302	4,208169594
567	--	6,216	-2767,58839	0,155400302	4,228659778
568	--	6,477	-2767,58761	0,156176001	4,249767634
569	--	6,739	-2767,58722	0,156569101	4,260464435
570	--	7	-2767,58705	0,156741802	4,265163871

Table S8. Summary of Morse potential calculations for **PdP**.

Entry	Charge	M···N (Å)	*E* (hartree)	Δ*E* (hartree)	Δ*E* (eV)
571	++	2,034	-1115,67656	0	0
572	++	2,295	-1115,53982	0,136734301	3,720731758
573	++	2,557	-1115,45802	0,2185339	5,946613366
574	++	2,818	-1115,40609	0,270464601	7,359720444
575	++	3,079	-1115,38354	0,2930163	7,973383746
576	++	3,341	-1115,37078	0,305778401	8,320658381
577	++	3,602	-1115,36372	0,312836401	8,512716442
578	++	3,864	-1115,3582	0,318356501	8,662926091
579	++	4,125	-1115,35387	0,322686801	8,780759617
580	++	4,386	-1115,35075	0,3258084	8,865702696
581	++	4,648	-1115,34853	0,3280215	8,925924245
582	++	4,909	-1115,34702	0,329535101	8,967111447

583	++	5,17	-1115,34595	0,3306078	8,996301089
584	++	5,432	-1115,34524	0,331318	9,015626625
585	++	5,693	-1115,34413	0,332423801	9,045717019
586	++	5,955	-1115,3444	0,332152	9,038320933
587	++	6,216	-1115,34426	0,3322937	9,042176788
588	++	6,477	-1115,34415	0,332402	9,045123783
589	++	6,739	-1115,31142	0,365134601	9,935823682
590	++	7	-1115,32012	0,3564349	9,699092638
591	+	2,034	-1116,05496	0	0
592	+	2,295	-1115,93919	0,115769101	3,150239315
593	+	2,557	-1115,88054	0,174418801	4,746179762
594	+	2,818	-1115,84415	0,210812202	5,736495154
595	+	3,079	-1115,81375	0,2412096	6,563650909
596	+	3,341	-1115,78731	0,267655902	7,283291812
597	+	3,602	-1115,76708	0,287885601	7,833770243
598	+	3,864	-1115,75267	0,302292101	8,225791277
599	+	4,125	-1115,74441	0,310548201	8,450451317
600	+	4,386	-1115,74254	0,312422501	8,501453644
601	+	4,648	-1115,73607	0,318892501	8,677511402
602	+	4,909	-1115,73589	0,319070801	8,682363194
603	+	5,17	-1115,7341	0,320859902	8,731047137
604	+	5,432	-1115,73067	0,3242885	8,824344089
605	+	5,693	-1115,73033	0,324635601	8,833789193
606	+	5,955	-1115,73002	0,324941602	8,842115909
607	+	6,216	-1115,72988	0,3250864	8,846056065
608	+	6,477	-1115,73017	0,324791402	8,838028756
609	+	6,739	-1115,71195	0,3430096	9,333771429
610	+	7	-1115,71929	0,335668201	9,134001685
611	0	2,034	-1116,30116	0	0
612	0	2,295	-1116,19275	0,108413199	2,950074923
613	0	2,557	-1116,07738	0,223777199	6,089290873
614	0	2,818	-1116,03903	0,2621326	7,132995032
615	0	3,079	-1116,02234	0,278819699	7,587074357
616	0	3,341	-1116,01321	0,287955899	7,83568315
617	0	3,602	-1116,0079	0,2932647	7,980143058
618	0	3,864	-1116,00383	0,297331499	8,090806352
619	0	4,125	-1116,00102	0,3001373	8,167156125
620	0	4,386	-1115,99877	0,3023939	8,22856137
621	0	4,648	-1115,99725	0,3039128	8,269892766
622	0	4,909	-1115,99608	0,3050816	8,30169745
623	0	5,17	-1115,99576	0,3054053	8,31050578
624	0	5,432	-1115,99488	0,3062812	8,334340246
625	0	5,693	-1115,99435	0,306816	8,348892902
626	0	5,955	-1115,99415	0,307008499	8,35413107
627	0	6,216	-1115,9937	0,307460999	8,366444228

628	0	6,477	-1115,99347	0,307688199	8,372626658
629	0	6,739	-1115,9934	0,3077599	8,374577743
630	0	7	-1115,98736	0,313804099	8,53904886
631	-	2,034	-1116,34548	0	0
632	-	2,295	-1116,26889	0,076582601	2,083919797
633	-	2,557	-1116,2095	0,135973601	3,700032046
634	-	2,818	-1116,16096	0,184513301	5,020865239
635	-	3,079	-1116,10001	0,245462801	6,679386463
636	-	3,341	-1116,11563	0,229842301	6,254330789
637	-	3,602	-1116,08786	0,2576122	7,009988619
638	-	3,864	-1116,08237	0,263107201	7,159515289
639	-	4,125	-1116,07875	0,266729601	7,258085865
640	-	4,386	-1116,07616	0,269312602	7,328372938
641	-	4,648	-1116,07319	0,272287101	7,40931322
642	-	4,909	-1116,07107	0,274403201	7,466895264
643	-	5,17	-1116,07148	0,274000902	7,455948145
644	-	5,432	-1116,0706	0,2748737	7,4796982
645	-	5,693	-1116,06905	0,2764234	7,521867707
646	-	5,955	-1116,06953	0,275943302	7,508803568
647	-	6,216	-1116,06917	0,2763106	7,518798261
648	-	6,477	-1116,06776	0,277715702	7,557033053
649	-	6,739	-1116,05573	0,289742801	7,884307255
650	-	7	-1116,06325	0,282221401	7,679639431
651	--	2,034	-1116,25605	0	0
652	--	2,295	-1116,178	0,078054601	2,123974978
653	--	2,557	-1116,11144	0,144613601	3,935138542
654	--	2,818	-1116,10204	0,1540149	4,19096105
655	--	3,079	-1116,09054	0,1655166	4,503938409
656	--	3,341	-1116,08063	0,175428702	4,773660582
657	--	3,602	-1116,07346	0,1825922	4,968589391
658	--	3,864	-1116,06755	0,1885022	5,129408765
659	--	4,125	-1116,06321	0,1928402	5,247451818
660	--	4,386	-1116,05997	0,196080901	5,335635829
661	--	4,648	-1116,05719	0,1988644	5,411378734
662	--	4,909	-1116,05472	0,2013312	5,478503816
663	--	5,17	-1116,05475	0,201304302	5,477771883
664	--	5,432	-1116,05355	0,2025044	5,51042823
665	--	5,693	-1116,05246	0,203593701	5,540069635
666	--	5,955	-1116,05225	0,203806002	5,545846643
667	--	6,216	-1116,05172	0,2043324	5,560170669
668	--	6,477	-1116,0508	0,2052573	5,585338493
669	--	6,739	-1116,02789	0,2281652	6,208694523
670	--	7	-1116,02959	0,2264599	6,162290923

Table S9. Summary of Morse potential calculations for **PtP**.

Entry	Charge	M···N (Å)	*E* (hartree)	Δ*E* (hartree)	Δ*E* (eV)
671	++	2,027	-1107,15743	0	0
672	++	2,289	-1107,00943	0,1479978	4,027227335
673	++	2,55	-1106,89388	0,263545899	7,171452876
674	++	2,812	-1106,81575	0,3416823	9,297653738
675	++	3,074	-1106,78484	0,372592499	10,13876353
676	++	3,336	-1106,76768	0,389746999	10,60556149
677	++	3,597	-1106,75834	0,3990863	10,85969694
678	++	3,859	-1106,75302	0,404408399	11,00451871
679	++	4,121	-1106,74886	0,408565199	11,11763106
680	++	4,383	-1106,74578	0,411650799	11,20159455
681	++	4,644	-1106,7437	0,4137257	11,25805551
682	++	4,906	-1106,74219	0,4152376	11,29919643
683	++	5,168	-1106,74114	0,416287199	11,32775749
684	++	5,43	-1106,74034	0,417089999	11,3496028
685	++	5,691	-1106,73326	0,4241722	11,5423194
686	++	5,953	-1106,73925	0,4181778	11,37920339
687	++	6,215	-1106,73283	0,424594	11,55379717
688	++	6,477	-1106,64377	0,5136535	13,97723085
689	++	6,738	-1106,72617	0,431259299	11,73516929
690	++	7	-1106,73928	0,4181486	11,37840881
691	+	2,027	-1107,53992	0	0
692	+	2,289	-1107,41844	0,1214804	3,305651757
693	+	2,55	-1107,26193	0,277994201	7,564611401
694	+	2,812	-1107,24966	0,2902562	7,898277561
695	+	3,074	-1107,21604	0,3238794	8,813211905
696	+	3,336	-1107,18646	0,353461999	9,61819584
697	+	3,597	-1107,16497	0,374953199	10,20300148
698	+	3,859	-1107,15148	0,388443001	10,57007788
699	+	4,121	-1107,14201	0,3979095	10,82767457
700	+	4,383	-1107,13741	0,402504999	10,95272453
701	+	4,644	-1107,13528	0,4046429	11,01089981
702	+	4,906	-1107,13439	0,4055332	11,03512612
703	+	5,168	-1107,13366	0,4062611	11,0549333
704	+	5,43	-1107,12844	0,4114761	11,19684075
705	+	5,691	-1107,13285	0,407072401	11,07700993
706	+	5,953	-1107,12804	0,4118842	11,20794572
707	+	6,215	-1107,12744	0,412482999	11,22423988
708	+	6,477	-1107,13241	0,4075101	11,08892034
709	+	6,738	-1107,12734	0,412578201	11,22683046
710	+	7	-1107,12728	0,412642499	11,2285801
711	0	2,027	-1107,78975	0	0
712	0	2,289	-1107,67118	0,1185661	3,226349574

713	0	2,55	-1107,50787	0,2818738	7,670180721
714	0	2,812	-1107,45221	0,337536499	9,184840689
715	0	3,074	-1107,43072	0,359028399	9,769665377
716	0	3,336	-1107,41924	0,3705044	10,08194343
717	0	3,597	-1107,4123	0,377442699	10,27074426
718	0	3,859	-1107,40727	0,3824751	10,40768294
719	0	4,121	-1107,40375	0,385997999	10,50354595
720	0	4,383	-1107,40132	0,3884278	10,56966424
721	0	4,644	-1107,39968	0,390066599	10,61425825
722	0	4,906	-1107,39836	0,391382899	10,65007662
723	0	5,168	-1107,39734	0,392403901	10,67785951
724	0	5,43	-1107,39664	0,3931011	10,69683127
725	0	5,691	-1107,39603	0,3937116	10,71344383
726	0	5,953	-1107,39559	0,394159699	10,72563723
727	0	6,215	-1107,39541	0,3943328	10,73034755
728	0	6,477	-1107,39515	0,3945961	10,73751232
729	0	6,738	-1107,39492	0,394830199	10,74388248
730	0	7	-1107,38353	0,406218	11,05376049
731	-	2,027	-1107,8309	0	0
732	-	2,289	-1107,72429	0,106606198	2,900903896
733	-	2,55	-1107,62701	0,203893099	5,548216674
734	-	2,812	-1107,51777	0,313127099	8,520626742
735	-	3,074	-1107,54145	0,2894485	7,876298913
736	-	3,336	-1107,52303	0,307863899	8,377407701
737	-	3,597	-1107,48943	0,3414653	9,291748864
738	-	3,859	-1107,48306	0,347838599	9,465175253
739	-	4,121	-1107,47809	0,352805499	9,600331555
740	-	4,383	-1107,47499	0,355911599	9,684852885
741	-	4,644	-1107,47266	0,358236499	9,748116669
742	-	4,906	-1107,47081	0,3600899	9,798550305
743	-	5,168	-1107,49833	0,332570199	9,049700713
744	-	5,43	-1107,46893	0,361969499	9,849696825
745	-	5,691	-1107,4968	0,334098199	9,091279732
746	-	5,953	-1107,46846	0,3624391	9,862475326
747	-	6,215	-1107,46817	0,362731099	9,870421027
748	-	6,477	-1107,46832	0,3625753	9,866181518
749	-	6,738	-1107,46821	0,362691	9,869329877
750	-	7	-1107,46752	0,363374099	9,887917958
751	--	2,027	-1107,73929	0	0
752	--	2,289	-1107,64999	0,089299601	2,429967152
753	--	2,55	-1107,52058	0,2187072	5,951329102
754	--	2,812	-1107,51265	0,226643801	6,167295127
755	--	3,074	-1107,4983	0,2409965	6,55785216
756	--	3,336	-1107,48663	0,252661601	6,875275889
757	--	3,597	-1107,47709	0,2621991	7,13480459

758	--	3,859	-1107,4699	0,269396301	7,330650505
759	--	4,121	-1107,46439	0,274901001	7,480441099
760	--	4,383	-1107,46071	0,278581601	7,580595377
761	--	4,644	-1107,45781	0,281485101	7,659603677
762	--	4,906	-1107,45549	0,283799201	7,722573578
763	--	5,168	-1107,45371	0,285583401	7,771124158
764	--	5,43	-1107,45276	0,286533602	7,796980457
765	--	5,691	-1107,45186	0,2874339	7,821478826
766	--	5,953	-1107,45062	0,2886749	7,855248174
767	--	6,215	-1107,4502	0,2890926	7,866614376
768	--	6,477	-1107,44976	0,2895333	7,87860644
769	--	6,738	-1107,44932	0,2899714	7,890527754
770	--	7	-1107,44919	0,290099502	7,894013589

3.4 XYZ files

Geometry optimized **MP**s:

ωB97X-D/def2-SVP(D)

FeP: -2250.987957 hartrees

	X	Y	Z
C	-1.090000	-0.001394	-2.828381
C	-0.678417	0.000595	-4.210438
H	-1.356367	0.000375	-5.060244
C	0.679020	0.002899	-4.210258
H	1.357247	0.004893	-5.059819
C	1.090309	0.002217	-2.828016
N	0.000097	-0.000512	-2.002356
C	2.412381	0.002872	-2.411941
H	3.182948	0.004568	-3.182413
C	2.828226	0.001077	-1.089978
C	4.210391	0.000173	-0.678357
H	5.060075	0.000664	-1.356465
C	4.210329	-0.001629	0.678998
H	5.059917	-0.002817	1.357191
C	2.827972	-0.001752	1.090324
N	2.002262	-0.000332	0.000292
C	2.412017	-0.001985	2.412376
H	3.182300	-0.002677	3.183126
C	-2.411985	-0.003447	-2.412219
H	-3.182569	-0.004873	-3.182706
C	-2.827941	-0.003098	-1.090264
C	1.089924	-0.000625	2.828039
C	0.678329	0.001549	4.210298
H	1.356465	0.001737	5.059947
C	-0.678972	0.002390	4.210275
H	-1.357297	0.003864	5.059774
C	-1.090369	0.001758	2.827903
N	-0.000149	0.000060	2.002109
C	-2.412331	0.001770	2.412172
H	-3.182965	0.003007	3.182578
C	-2.828241	0.000136	1.090032
N	-2.002228	-0.000841	0.000130
C	-4.210374	-0.001114	0.678415
H	-5.060053	-0.000123	1.356509
C	-4.210215	-0.003137	-0.678972
H	-5.059770	-0.004248	-1.357221
Fe	0.000036	-0.001998	-0.000442

ωB97X-D/6-31G(d)

FeP: -2251.657005 hartrees

	X	Y	Z
C	-1.088922	0.018112	2.821478
C	-0.676624	0.025490	4.200219
H	-1.352534	0.034527	5.045305
C	0.677553	0.017578	4.200005
H	1.354246	0.018433	5.044520
C	1.089500	0.005691	2.821249
N	0.000212	0.008970	1.987322
C	2.408662	-0.010125	2.408118
H	3.176451	-0.015164	3.175433
C	2.821342	-0.017322	1.088810
C	4.200050	-0.022491	0.676478
H	5.044713	-0.029442	1.352975
C	4.200043	-0.015615	-0.677703
H	5.045487	-0.015664	-1.353281
C	2.821387	-0.005436	-1.089745
N	1.987188	-0.008859	-0.000637
C	2.408390	0.009813	-2.409032
H	3.175740	0.014941	-3.176800
C	-2.408358	0.009854	2.408856
H	-3.175602	0.014803	3.176725
C	-2.821557	-0.006734	1.089790
C	1.089035	0.017345	-2.821552
C	0.676513	0.024643	-4.200212
H	1.352542	0.032748	-5.045282
C	-0.677562	0.018337	-4.200095
H	-1.354255	0.020241	-5.044588
C	-1.089523	0.006379	-2.821122
N	-0.000127	0.008779	-1.987235
C	-2.408578	-0.009977	-2.408045
H	-3.176380	-0.015026	-3.175322
C	-2.821300	-0.018693	-1.088703
N	-1.987422	-0.009658	0.000613
C	-4.200247	-0.027178	-0.676419
H	-5.044311	-0.036539	-1.353588
C	-4.200303	-0.019844	0.677666
H	-5.045265	-0.021928	1.353815
Fe	-0.000188	-0.000989	-0.000015

ωB97X-D/def2-SVP(D)

CoP: -2370.093142 hartrees

	X	Y	Z
C	-1.087752	0.000000	-2.816709
C	-0.678267	0.000000	-4.197730
H	-1.356918	0.000000	-5.046976
C	0.678267	0.000000	-4.197730
H	1.356918	0.000000	-5.046976
C	1.087752	0.000000	-2.816709
N	0.000000	0.000000	-1.986633
C	2.409918	0.000000	-2.409551
H	3.179395	0.000000	-3.181111
C	2.818520	0.000000	-1.088402
C	4.199209	0.000000	-0.677407
H	5.049406	0.000000	-1.353334
C	4.198209	0.000000	0.678524
H	5.045889	0.000000	1.358515
C	2.816698	0.000000	1.086844
N	1.987528	0.000000	-0.000650
C	2.408984	0.000000	2.408690
H	3.179821	0.000000	3.178931
C	-2.409918	0.000000	-2.409551
H	-3.179395	0.000000	-3.181111
C	-2.818520	0.000000	-1.088402
C	1.087679	0.000000	2.816479
C	0.677703	0.000000	4.197580
H	1.355765	0.000000	5.045785
C	-0.677703	0.000000	4.197580
H	-1.355765	0.000000	5.045785
C	-1.087679	0.000000	2.816479
N	0.000000	0.000000	1.986583
C	-2.408984	0.000000	2.408690
H	-3.179821	0.000000	3.178931
C	-2.816698	0.000000	1.086844
N	-1.987528	0.000000	-0.000650
C	-4.198209	0.000000	0.678524
H	-5.045889	0.000000	1.358515
C	-4.199209	0.000000	-0.677407
H	-5.049406	0.000000	-1.353334
Co	0.000000	0.000000	0.001094

ωB97X-D/6-31G(d)

CoP: -2370.669193 hartrees

	X	Y	Z
C	1.085621	-0.000330	2.791328
C	0.671021	-0.000233	4.183357
H	1.355503	-0.000465	5.021230
C	-0.671020	0.000232	4.183357
H	-1.355503	0.000465	5.021230
C	-1.085620	0.000330	2.791326
N	-0.000002	-0.000000	1.939219
C	-2.405485	0.000580	2.405339
H	-3.171751	0.000827	3.172481
C	-2.792034	0.000332	1.085728
C	-4.184183	0.000241	0.670370
H	-5.023231	0.000476	1.353572
C	-4.183390	-0.000225	-0.671751
H	-5.020584	-0.000450	-1.357333
C	-2.791210	-0.000333	-1.085115
N	-1.939364	-0.000001	0.000516
C	-2.404954	-0.000592	-2.404634
H	-3.171689	-0.000853	-3.171201
C	2.405485	-0.000580	2.405339
H	3.171751	-0.000827	3.172481
C	2.792037	-0.000332	1.085730
C	-1.085444	-0.000334	-2.790818
C	-0.671050	-0.000231	-4.182924
H	-1.355849	-0.000457	-5.020676
C	0.671050	0.000231	-4.182925
H	1.355849	0.000456	-5.020676
C	1.085442	0.000334	-2.790816
N	0.000002	0.000000	-1.938608
C	2.404954	0.000592	-2.404635
H	3.171690	0.000853	-3.171201
C	2.791208	0.000334	-1.085114
N	1.939364	0.000001	0.000512
C	4.183391	0.000225	-0.671750
H	5.020584	0.000449	-1.357332
C	4.184182	-0.000240	0.670371
H	5.023231	-0.000476	1.353572
Co	0.000000	0.000000	0.000448

ωB97X-D/def2-SVP(D)

NiP: -2495.629943 hartrees

	X	Y	Z
C	-1.084772	0.016225	-2.805838
C	-0.677293	0.015911	-4.186140
H	-1.359856	0.024297	-5.031935
C	0.678078	0.000045	-4.186013
H	1.360784	-0.006854	-5.031631
C	1.085470	-0.007635	-2.805451
N	0.000083	0.002200	-1.972127
C	2.405884	-0.022499	-2.405518
H	3.176635	-0.032162	-3.175185
C	2.805391	-0.016995	-1.084553
C	4.185632	-0.014231	-0.677286
H	5.031882	-0.022746	-1.359763
C	4.185762	0.003413	0.677992
H	5.031671	0.011794	1.360156
C	2.805342	0.009184	1.085581
N	1.971564	-0.003600	0.000694
C	2.405631	0.022765	2.406227
H	3.175296	0.033927	3.176741
C	-2.405263	0.022014	-2.406060
H	-3.175119	0.031488	-3.175770
C	-2.805091	0.010164	-1.085585
C	1.084858	0.016649	2.805895
C	0.677475	0.013984	4.186234
H	1.360619	0.026845	5.032192
C	-0.678783	-0.005472	4.185974
H	-1.361769	-0.012285	5.031225
C	-1.085780	-0.011729	2.805566
N	-0.000305	0.000885	1.971787
C	-2.406419	-0.024044	2.405752
H	-3.176635	-0.032535	3.175632
C	-2.805556	-0.017300	1.084627
N	-1.971658	-0.002824	-0.000385
C	-4.185947	-0.015352	0.677125
H	-5.031324	-0.027982	1.360131
C	-4.185634	0.003374	-0.678516
H	-5.030862	0.011465	-1.361797
Ni	0.000008	-0.000386	0.000025

ωB97X-D/6-31G(d)

NiP: -2496.267948 hartrees

	X	Y	Z
C	-1.063735	0.212459	-2.775145
C	-0.659285	0.152351	-4.152228
H	-1.325527	0.294491	-4.992644
C	0.661365	-0.141953	-4.152352
H	1.328494	-0.278688	-4.992980
C	1.064574	-0.210567	-2.775362
N	0.000297	-0.000526	-1.935495
C	2.373506	-0.360328	-2.373428
H	3.132179	-0.517166	-3.132602
C	2.775532	-0.210986	-1.064435
C	4.152397	-0.146016	-0.660516
H	4.993289	-0.285726	-1.327002
C	4.152459	0.144013	0.660830
H	4.993087	0.281415	1.327969
C	2.775732	0.209739	1.064656
N	1.935886	-0.000042	-0.000104
C	2.373402	0.358155	2.373611
H	3.132162	0.516403	3.132381
C	-2.373140	0.359579	-2.373358
H	-3.131810	0.520699	-3.131840
C	-2.775491	0.205677	-1.065158
C	1.064540	0.209856	2.775563
C	0.660179	0.147386	4.152704
H	1.326409	0.286644	4.993668
C	-0.661498	-0.141467	4.152817
H	-1.328757	-0.277571	4.993767
C	-1.065244	-0.207959	2.775770
N	-0.000410	0.000065	1.935948
C	-2.374016	-0.358839	2.373507
H	-3.132994	-0.516589	3.132423
C	-2.775511	-0.214164	1.064138
N	-1.935680	-0.004513	-0.000762
C	-4.152407	-0.151687	0.659610
H	-4.993520	-0.290080	1.326119
C	-4.152631	0.138716	-0.661853
H	-4.993717	0.278548	-1.328017
Ni	-0.000116	-0.001327	-0.000198

ωB97X-D/def2-SVP(D)

CuP: -2627.765231 hartrees

	X	Y	Z
C	-1.091829	-0.002977	-2.835364
C	-0.679117	-0.000237	-4.218118
H	-1.355371	-0.003435	-5.069394
C	0.679360	0.005426	-4.218408
H	1.356074	0.009027	-5.069233
C	1.092628	0.006415	-2.835963
N	0.000599	0.001698	-2.017748
C	2.415140	0.008396	-2.414931
H	3.186062	0.012384	-3.185107
C	2.835617	0.003719	-1.092232
C	4.218178	0.001396	-0.679226
H	5.069422	0.003932	-1.355211
C	4.218067	-0.005093	0.679297
H	5.069352	-0.009410	1.355634
C	2.835268	-0.005645	1.092085
N	2.017469	-0.001069	-0.000158
C	2.414915	-0.007086	2.414696
H	3.185519	-0.010843	3.185180
C	-2.414469	-0.008155	-2.414788
H	-3.184690	-0.012280	-3.185748
C	-2.835773	-0.006568	-1.092302
C	1.092191	-0.002517	2.835851
C	0.679324	-0.000101	4.218521
H	1.355103	-0.002473	5.069971
C	-0.679287	0.004996	4.218181
H	-1.356373	0.007980	5.068927
C	-1.092256	0.005720	2.835571
N	0.000521	0.001349	2.017853
C	-2.414756	0.007107	2.414817
H	-3.185344	0.010621	3.185456
C	-2.836161	0.002634	1.092347
N	-2.018131	-0.001415	0.000029
C	-4.218502	-0.000226	0.679189
H	-5.069306	0.002844	1.355777
C	-4.218385	-0.006673	-0.679314
H	-5.069296	-0.010573	-1.356267
Cu	-0.001765	0.001129	0.000129

ωB97X-D/6-31G(d)

CuP: -2628.402655 hartrees

	X	Y	Z
C	-2.825899	1.090646	0.000640
C	-4.204816	0.677815	0.000285
H	-5.050234	1.353385	-0.000283
C	-4.204752	-0.677348	-0.000644
H	-5.050179	-1.352864	-0.001948
C	-2.825358	-1.089514	0.000535
N	-1.997808	0.000488	0.001176
C	-2.409717	-2.409448	-0.000251
H	-3.177358	-3.176828	-0.000686
C	-1.089917	-2.825382	-0.000300
C	-0.677497	-4.204541	-0.000370
H	-1.353060	-5.049925	-0.000829
C	0.677711	-4.204614	-0.000218
H	1.353249	-5.050084	-0.000416
C	1.090047	-2.825451	0.000908
N	0.000495	-1.997456	-0.000286
C	2.410061	-2.410038	0.002080
H	3.177553	-3.177489	0.002076
C	-2.409455	2.410133	-0.000205
H	-3.176212	3.178304	-0.000207
C	-1.089110	2.824742	-0.000663
C	2.825109	-1.090109	0.002046
C	4.204240	-0.677601	-0.000312
H	5.049519	-1.353353	-0.001413
C	4.204446	0.677471	-0.000580
H	5.049735	1.353125	-0.002058
C	2.824970	1.089481	0.001055
N	1.996797	0.000105	0.001995
C	2.410276	2.409732	0.000217
H	3.178282	3.176747	-0.000483
C	1.090694	2.825604	-0.000507
N	0.000915	1.997113	-0.000831
C	0.677785	4.204692	-0.001762
H	1.353305	5.050106	-0.002544
C	-0.677278	4.204240	-0.000858
H	-1.353241	5.049331	-0.001002
Cu	-0.003296	-0.001217	0.006645

ωB97X-D/def2-SVP(D)

ZnP: -2766.647305 hartrees

	X	Y	Z
C	-1.096728	0.003126	-2.857663
C	-0.680531	0.005129	-4.242028
H	-1.352700	0.009186	-5.096471
C	0.679866	-0.004322	-4.241962
H	1.351348	-0.004603	-5.097121
C	1.096994	-0.008811	-2.858118
N	0.000386	-0.004380	-2.048665
C	2.420966	-0.011550	-2.421593
H	3.191681	-0.015627	-3.192886
C	2.858496	-0.007082	-1.097824
C	4.242898	-0.003213	-0.680471
H	5.098102	-0.005163	-1.351724
C	4.242343	0.009011	0.680196
H	5.096975	0.012542	1.352181
C	2.857689	0.008331	1.096488
N	2.048996	-0.002840	-0.000787
C	2.420335	0.011436	2.420144
H	3.191730	0.017309	3.190940
C	-2.420412	0.008194	-2.419967
H	-3.190749	0.011984	-3.192145
C	-2.858008	0.006331	-1.096622
C	1.096844	0.003514	2.857373
C	0.680402	0.000582	4.241719
H	1.352332	0.003306	5.096649
C	-0.680377	-0.005551	4.242074
H	-1.351735	-0.009161	5.097287
C	-1.097439	-0.005500	2.858047
N	-0.000385	-0.000794	2.048567
C	-2.421169	-0.010122	2.421399
H	-3.192228	-0.014640	3.192172
C	-2.857970	-0.006139	1.097443
N	-2.048825	0.001410	0.000597
C	-4.242393	-0.003534	0.680803
H	-5.097305	-0.003416	1.352970
C	-4.242263	0.006731	-0.679735
H	-5.097113	0.011495	-1.351398
Zn	-0.000053	-0.003168	0.000135

ωB97X-D/6-31G(d)

ZnP: -2767.246579 hartrees

	X	Y	Z
C	-1.094771	-0.001134	-2.850529
C	-0.678106	-0.000712	-4.231873
H	-1.348597	0.001264	-5.081438
C	0.679252	-0.002899	-4.232283
H	1.348886	-0.003885	-5.082564
C	1.096750	-0.004934	-2.851281
N	0.001605	-0.003705	-2.034618
C	2.417777	-0.004656	-2.417098
H	3.186433	-0.006526	-3.184254
C	2.850067	-0.000257	-1.095323
C	4.231442	0.000934	-0.678084
H	5.081325	-0.001562	-1.348282
C	4.231196	0.004742	0.679234
H	5.081312	0.006871	1.348901
C	2.849857	0.004456	1.095940
N	2.033450	0.002592	0.000127
C	2.417020	0.003307	2.417316
H	3.185583	0.004013	3.184810
C	-2.416256	0.001570	-2.417356
H	-3.183680	0.002202	-3.185961
C	-2.851024	0.003968	-1.096378
C	1.095826	0.000785	2.851245
C	0.678419	-0.005281	4.232413
H	1.348825	-0.008415	5.082119
C	-0.679070	-0.006112	4.231946
H	-1.348651	-0.009843	5.082325
C	-1.095816	-0.001113	2.850720
N	0.000532	0.002190	2.034717
C	-2.417045	0.001016	2.416799
H	-3.184739	-0.001789	3.184709
C	-2.851161	0.003690	1.095549
N	-2.034908	0.006404	-0.000385
C	-4.232097	0.000982	0.678187
H	-5.081813	-0.001751	1.348795
C	-4.231944	0.001718	-0.679331
H	-5.082075	-0.000200	-1.349282
Zn	-0.003802	0.012070	0.000467

ωB97X-D/def2-SVP(D)

PdP: -1115.364794 hartrees

	X	Y	Z
C	-1.096021	0.000044	-2.840470
C	-0.678814	0.000073	-4.222145
H	-1.355032	-0.000139	-5.073409
C	0.679158	0.000923	-4.222177
H	1.355479	0.001677	-5.073453
C	1.096435	0.000608	-2.840483
N	0.000095	-0.000049	-2.028796
C	2.417491	0.000848	-2.417114
H	3.188233	0.001959	-3.187717
C	2.840639	0.000326	-1.096005
C	4.222261	0.001486	-0.678815
H	5.073586	0.002542	-1.355028
C	4.222070	0.001789	0.678627
H	5.073216	0.002765	1.354710
C	2.840418	-0.000015	1.096177
N	2.028736	-0.000789	0.000018
C	2.416951	-0.000418	2.417222
H	3.187439	0.000006	3.187862
C	-2.416849	0.000453	-2.417002
H	-3.187313	0.000797	-3.187451
C	-2.840235	0.000377	-1.095993
C	1.095970	-0.001327	2.840464
C	0.678526	-0.001597	4.222108
H	1.354590	-0.001528	5.073388
C	-0.679375	-0.001359	4.222091
H	-1.355896	-0.000817	5.073352
C	-1.096311	-0.001737	2.840378
N	-0.000001	-0.001850	2.028703
C	-2.417359	-0.001463	2.416987
H	-3.188184	-0.001065	3.187648
C	-2.840585	-0.000981	1.095943
N	-2.028651	0.000075	-0.000094
C	-4.222210	-0.000870	0.678799
H	-5.073565	-0.001145	1.354978
C	-4.221912	0.000366	-0.678605
H	-5.073019	0.001003	-1.354655
Pd	0.000040	-0.000968	-0.000042

ωB97X-D/6-31G(d)

PdP: -1114.835172 hartrees

	X	Y	Z
C	1.098606	0.000606	2.844423
C	0.677589	-0.004250	4.223573
H	1.350848	-0.005479	5.070683
C	-0.677865	-0.009040	4.223380
H	-1.349523	-0.014337	5.071798
C	-1.098330	-0.003899	2.844217
N	0.000620	0.001180	2.033924
C	-2.416832	-0.002348	2.417100
H	-3.184408	-0.005191	3.184529
C	-2.844229	0.002106	1.098052
C	-4.223393	0.004004	0.678038
H	-5.070709	0.002751	1.351064
C	-4.223737	0.006620	-0.677678
H	-5.071628	0.008426	-1.349945
C	-2.844872	0.006160	-1.098659
N	-2.034296	0.003470	-0.000392
C	-2.417769	0.004814	-2.417678
H	-3.185379	0.006604	-3.185062
C	2.417639	0.004683	2.417414
H	3.184976	0.006201	3.185082
C	2.844537	0.005721	1.098707
C	-1.099055	0.000682	-2.844739
C	-0.677730	-0.004941	-4.223755
H	-1.349590	-0.006085	-5.071917
C	0.677842	-0.009045	-4.223313
H	1.350584	-0.013967	-5.070896
C	1.097720	-0.005160	-2.844119
N	-0.000583	0.000107	-2.034127
C	2.416718	-0.004126	-2.416710
H	3.183988	-0.007604	-3.184497
C	2.844126	0.000610	-1.098314
N	2.033951	0.002528	0.000437
C	4.223449	0.004204	-0.677700
H	5.071363	0.003808	-1.349950
C	4.223728	0.006076	0.677650
H	5.072076	0.008126	1.349414
Pd	-0.000434	0.005981	-0.000035

ωB97X-D/def2-SVP(D)

PtP: -1106.870851 hartrees

	X	Y	Z
C	-1.098004	0.001067	-2.843200
C	-0.677883	0.003716	-4.223565
H	-1.353434	0.004516	-5.074578
C	0.679041	0.003704	-4.223739
H	1.354775	0.004224	-5.074883
C	1.098388	0.002898	-2.843371
N	0.000202	0.001522	-2.029908
C	2.417589	0.001853	-2.417797
H	3.187791	0.001618	-3.188015
C	2.843038	0.000875	-1.098247
C	4.223420	-0.000271	-0.678362
H	5.074499	-0.000288	-1.353846
C	4.223463	-0.002455	0.679351
H	5.074692	-0.004072	1.355572
C	2.843021	-0.001290	1.098261
N	2.029713	-0.000983	0.000121
C	2.417698	-0.000488	2.417546
H	3.188245	-0.001305	3.187940
C	-2.417952	-0.001909	-2.417929
H	-3.188324	-0.002214	-3.188242
C	-2.843447	-0.002555	-1.098567
C	1.097901	0.001045	2.843033
C	0.678572	0.001067	4.223485
H	1.354583	0.000063	5.074513
C	-0.678402	0.000945	4.223588
H	-1.353656	-0.000426	5.074714
C	-1.098453	0.002421	2.843344
N	-0.000865	0.003499	2.029801
C	-2.417704	0.001167	2.417935
H	-3.187458	-0.001301	3.188141
C	-2.843335	-0.000923	1.098090
N	-2.030067	-0.000846	-0.000223
C	-4.223755	-0.002758	0.678475
H	-5.074889	-0.002774	1.354492
C	-4.223845	-0.003720	-0.679089
H	-5.074984	-0.004413	-1.354779
Pt	-0.000175	-0.001210	-0.000061

ωB97X-D/6-31G(d)

PtP: -1107.276084 hartrees

	X	Y	Z
C	2.841871	-0.001402	1.098852
C	4.219498	-0.002749	0.676007
H	5.067294	-0.003631	1.347909
C	4.219011	-0.002754	-0.678596
H	5.064937	-0.003598	-1.353029
C	2.841640	-0.001453	-1.099779
N	2.027410	-0.000986	-0.000475
C	2.416479	0.000018	-2.417052
H	3.184332	0.000853	-3.184197
C	1.099696	0.000728	-2.842766
C	0.678189	0.001315	-4.220506
H	1.351241	0.001183	-5.067948
C	-0.676414	0.001181	-4.219995
H	-1.348885	0.001689	-5.067498
C	-1.098225	0.000490	-2.842110
N	0.000788	0.000395	-2.027799
C	-2.415025	-0.000217	-2.415824
H	-3.182121	-0.001301	-3.183763
C	2.415609	0.000063	2.416161
H	3.183555	0.000970	3.183023
C	1.098953	0.000796	2.843621
C	-2.841938	0.000006	-1.098683
C	-4.219990	-0.000213	-0.677235
H	-5.067737	0.000293	-1.349654
C	-4.220529	-0.000216	0.677310
H	-5.068706	0.000016	1.349018
C	-2.842968	0.000066	1.099783
N	-2.028148	0.000367	0.000871
C	-2.416866	-0.000022	2.417008
H	-3.185086	-0.001053	3.183824
C	-1.099858	0.000614	2.843759
N	-0.000480	0.000504	2.029413
C	-0.677689	0.001161	4.221317
H	-1.349408	0.001446	5.069394
C	0.676933	0.001250	4.221318
H	1.348659	0.001069	5.069395
Pt	-0.000499	0.000100	0.000524

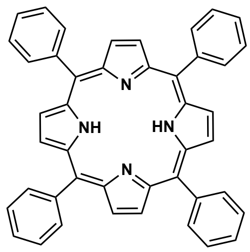
4 Synthetic Section

4.1 General Information

Chemicals were purchased from Sigma-Aldrich and used without any further purification. CH_2Cl_2 was neutralized with K_2CO_3 and distilled prior to usage. Reactions were carried out in darkness and under a dry argon atmosphere, using standard Schlenk techniques. Reaction vessels were heated with polymer-coated heat-on blocks from Radleys. Thin layer chromatography (TLC) was performed on Merck silica gel 60 F_{254}, detected by UV light (254 nm & 365 nm). Gravimetrical and flash column chromatography were performed on silica gel 60 M (70–230 mesh, 0.063-0.200 mm). Automated column chromatography was conducted on Multiple Preparative HPLC LC-forte/R using 25-gram solid sample RediSep cartridges from Teledyne Isco, Inc. Nuclear magnetic resonance (NMR) spectroscopy was performed on a Bruker Avance III HD 300 (^{1}H: 300 MHz); Deuterated solvents were purchased from Sigma Aldrich and used as received. Chemical shifts are referenced to residual protic solvent peaks or to the deuterated solvent itself (δ in parts per million (ppm): $CHCl_3$: ^{1}H: 7.26 ppm, CH_3OD: ^{1}H: 3.31 ppm. The resonance multiplicities are indicated as "s" (singlet), "d" (doublet), "t" (triplet), "q" (quartet), and "m" (multiplet). Signals referred to as "b" (broad singlet) are not clearly resolved or significantly broadened. Matrix-assisted laser desorption ionization time-of-flight (MALDI-TOF) mass spectrometry (MS) was performed on a Bruker Autoflex Max spectrometer using (*E*)-2-(3(4-(*tert*-butyl)phenyl)-2-methylallylidene)-malononitrile (DCTB) as the matrix. Vibrational (IR) spectroscopy was performed on an Agilent Cary 630 F spectrometer using the attenuated total reflection (ATR) mode over the scanning range of 500-4000 cm^{-1}. The ATR unit was equipped with a diamond crystal plate and a high-pressure clamp. Spectra were recorded as solid samples directly from the diamond crystal. All absorptions $\tilde{\nu}$ are given in wave numbers [cm^{-1}]. Peak assignments were conducted according to literature-known assignments. Absorption (UV/Vis) spectroscopy was carried out on a Jasco V-770 spectrophotometer. Spectra were recorded at room temperature using quartz cuvettes with a light-path length of 1 cm. IR and UV/Vis data were analyzed using spectragryph 1.2.15 and Microsoft Excel 16.59. Melting points were measured using a calibrated BÜCHI M-565 at a heating rate of 1°C per minute. Standard deviations were determined from three samples through the implemented melting point analysis software from BÜCHI.

4.2 Synthetic Details

4.2.1 5,10,15,20-Tetraphenylporphyrin (**TPP**)



TPP
$C_{44}H_{30}N_4$
614.75 g/mol

A 2 L schlenk round bottom flask equipped with a magnetic stir bar and reflux condenser was charged with CH_2Cl_2 (1.5 L) and deoxygenated by passing a stream of argon through the solution for 1 h. Thereafter, pyrrole (1.0 mL, 15.0 mmol) and benzaldehyde (1.5 mL, 15.0 mmol) were added and the mixture was deoxygenated for another 15 min, before adding $BF_3{\cdot}OEt_2$ (185 µL, 1.5 mmol). The reaction was stirred in darkness under Ar for 2 h at rt. Subsequently, *para*-chloranil (2.8 g, 11.3 mmol) was added and the mixture was heated (70 °C) to reflux for 2 h. The reaction mixture was allowed to cool to rt, plug filtered (SiO_2, 6.5 cm x 4.5 cm; CH_2Cl_2), and concentrated. The crude product was dissolved in CH_2Cl_2 (200 mL) and washed with 10% Na_2SO_3 (4 x 50 mL). The combined aqueous layer was extracted with CH_2Cl_2 (2 x 50 mL). The combined organic layer was further washed with 10% Na_2CO_3 (2 x 100 mL), concentrated, and purified by column chromatography (SiO_2; $CHCl_3$/Hex (2:1)). After precipitation from CH_2Cl_2 with MeOH, the product was isolated as a purple-colored solid in 38% (870 mg, 1.4 mmol) yield.

$\mathbf{R_f}$ (SiO_2; 1:1 CH_2Cl_2:Hex): 0.37.

Mp [°C]: > 400, lit[5] 450.4 ± 0.4.

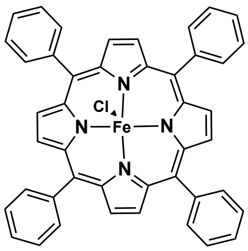
^{1}H NMR (300 MHz, $CDCl_3$, rt): δ [ppm] = 8.85 (s, 8H, **g**), 8.22 (d, ^3J = 7.7 Hz, 8H, **c**), 7.71 – 7.80 (m, 12H, **a,b**), -2.77 (s, 2H, **h**).

MS (MALDI-TOF, DCTB): *m/z* (rel. int.) = 614.164 $[M]^{+\bullet}$ (100%).

IR (ATR): υ_{max} [cm^{-1}]:3317, 3056, 2959, 1584, 1554, 1468, 1435, 1345, 954, 790, 690.

UV/Vis (CH_2Cl_2, rt): λ [nm] (ε [$M^{-1}cm^{-1}$]) = 417 (348000), 514 (13000), 548 (5100), 590 (3800), 647 (3500).

4.2.2 Chloro(5,10,15,20-tetraphenylporphyrinato) iron(III) (**FeTPP**)

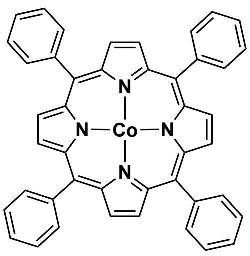


FeTPP
$C_{44}H_{28}FeN_4$
668.58 g/mol

A 100 mL round bottom flask equipped with a magnetic stir bar and a reflux condenser was charged with tetraphenylporphyrin (**TPP**) (100 mg, 163 µmol), 15 equiv. $FeCl_2$ (309 mg, 2.45 mmol), and dissolved in DMF (40 mL) in darkness under argon. The reaction was heated to reflux at 190 °C for 5 h and then stirred for 18 h under air at rt in darkness. The mixture was plug filtered (SiO_2, 6 cm x 5 cm; MeOH/Hex/EtOAc (1:1:1)), and concentrated. The crude was adsorbed on silica and purified by dry loading into a 25G Redisep cartridge for automated column chromatography (EtOAc/Hex (0/100 – 50/50)). The product was precipitated from MeOH with H_2O on the rotavapor to give a dark-brown colored solid in 64% (70 mg, 100 µmol) yield.

R_f (SiO_2; 1:1:2 CH_2Cl_2:EtOAc:Hex): 0.63.
Mp [ºC]: > 400, lit[6] > 300.
^{1}H NMR (300 MHz,CD_3OD, rt): δ [ppm] = [**FeTPP** is paramagnetic].
MS (MALDI-TOF, DCTB): *m/z (rel. int.)* = 668.220 $[M]^{+\bullet}$ (100%), 703.262 $[M+Cl]^{+\bullet}$ (26%).
IR (ATR): υ_{max} [cm^{-1}]: 2920, 2850, 1595, 1439, 1332, 1174, 1069, 994, 804, 748, 702, 656.
UV/Vis (CH_2Cl_2, rt): λ [nm] (ε [M^{-1}cm^{-1}]) = 336, (24000), 413 (65000), 619 (5000).

4.2.3 5,10,15,20-Tetraphenylporphyrinato cobalt(II) (**CoTPP**)

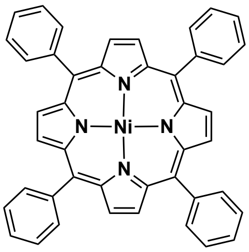


CoTPP
$C_{44}H_{28}CoN_4$
671.67 g/mol

A 100 mL round bottom flask equipped with a magnetic stir bar and a reflux condenser was charged with tetraphenylporphyrin (**TPP**) (100 mg, 163 µmol), 10 equiv. $Co(OAc)_2{\cdot}2H_2O$ (288 mg, 1.63 mmol), and dissolved in THF (50 mL). The mixture was heated in darkness under argon at 75 °C to reflux for 18 h. The mixture was cooled to rt, plug filtered (SiO_2, 6.5 cm 4.5 cm; 1:1 CH_2Cl_2/Hex), and precipitated from CH_2Cl_2 with MeOH, to give the product as a burgundy-colored solid in 57% (62 mg, 93 µmol) yield.

R_f (SiO_2; 1:1 CH_2Cl_2:Hex): 0.50.
Mp [ºC]: > 400, lit[5] 474.1 ± 0.8.
^{1}H NMR (300 MHz, $CDCl_3$, rt): δ [ppm] = 9.93 (b, **aromatic**), 9.73 (b, **aromatic**).
MS (MALDI-TOF, DCTB): *m/z (rel. int.)* = 671.280 $[M]^{+\bullet}$ (100%).
IR (ATR): υ_{max} [cm^{-1}]: 3048, 2849, 18,07, 11441, 1348, 1260, 1067, 1003, 794., 747, 654.
UV/Vis (CH_2Cl_2, rt): λ [nm] (ε [M^{-1}cm^{-1}]) = 410 (192000), 527 (11000).

4.2.4 5,10,15,20-Tetraphenylporphyrinato nickel(II) (**NiTPP**)



NiTPP
$C_{44}H_{28}N_4Ni$
671.43 g/mol

A 50 mL two-necked round bottom flask equipped with a magnetic stir bar and a reflux condenser was charged with tetraphenylporphyrin (**TPP**) (50 mg, 81.3 μmol), 10 equiv. of $Ni(OAc)_2$ (209 mg, 813 μmol), dissolved in toluene (25 mL) in darkness under argon, and heated to 135 °C to reflux for 24 h. The mixture was purified by plug filtration (SiO_2, 6 cm x 3 cm; toluene), concentrated, and precipitated from toluene with MeOH. The solid was filtered, washed with MeOH and dried in vacuum, to yield the product as purple solid in 46% (25 mg, 37.2 μmol) yield.

R_f (SiO_2; 1:1 CH_2Cl_2:Hex): 0.62.

Mp [ºC]: > 400, lit[5] 487 ± 0.4.

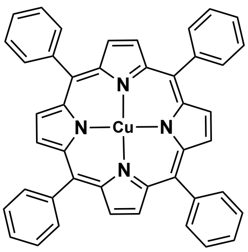
^{1}H NMR (300 MHz, $CDCl_3$, rt): δ [ppm] = 8.74 (s, 8H, **g**), 8.17 (d, ^3J = 7.8 Hz, 8H, **c**), 7.69 – 7.78 (m, 12H, **a,b**).

MS (MALDI-TOF, DCTB): *m/z (rel. int.)* = 670.281 $[M]^{+\bullet}$ (100%).

IR (ATR): υ_{max} [cm^{-1}]: 3052, 3022, 1440, 1350, 1245, 1177, 1006, 834, 791, 740, 694.

UV/Vis (CH_2Cl_2, rt): λ [nm] (ε [$M^{-1}cm^{-1}$]) = 414 (181000), 527 (17000).

4.2.5 5,10,15,20-Tetraphenylporphyrinato copper(II) (**CuTPP**)



CuTPP
$C_{44}H_{28}CuN_4$
676.28 g/mol

A 100 mL round bottom flask equipped with a magnetic stir bar was charged with tetraphenylporphyrin (**TPP**) (50 mg, 81.3 μmol) and dissolved in CH_2Cl_2 (50 mL). Then, a saturated solution of $Cu(OAc)_2 \cdot H_2O$ in MeOH (5 mL) was added. The mixture was stirred in darkness at rt for 18 h. The mixture was plug filtered (SiO_2, 6.5 cm x 4.5 cm; CH_2Cl_2) and concentrated. The crude product was adsorbed on silica and purified by dry loading into a 25G Redisep cartridge for automated column chromatography (SiO_2; CH_2Cl_2/Hex (0/100 – 50/50)). The product was precipitated from CH_2Cl_2 with MeOH to give a pink-colored solid in 97% (53 mg, 79 mmol) yield.

R_f (SiO_2; 1:1 CH_2Cl_2:Hex): 0.60.

Mp [ºC]: > 400, lit[5] 468.3 ± 0.7.

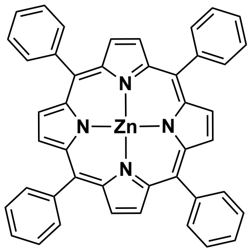
^{1}H NMR (300 MHz, $CDCl_3$, rt): δ [ppm] = 7.65 (b, **aromatic**), 7.50 (b, **aromatic**).

MS (MALDI-TOF, DCTB): *m/z (rel. Int.)* = 675.126 $[M]^{+\bullet}$ (100%).

IR (ATR): υ_{max} [cm^{-1}]: 3052, 3019, 1589, 1487, 1435, 1338, 1178, 995, 786, 697.

UV/Vis (CH_2Cl_2, rt): λ [nm] (ε [$M^{-1}cm^{-1}$]) = 414 (429000), 539 (15500).

4.2.6 5,10,15,20-Tetraphenylporphyrinato zinc(II) (**ZnTPP**)



ZnTPP
$C_{44}H_{28}ZnN_4$
678.12 g/mol

A 100 mL round bottom flask equipped with a magnetic stir bar was charged with tetraphenylporphyrin (**TPP**) (60 mg, 98 µmol) and dissolved in CH_2Cl_2 (50 mL). Then, a saturated solution of $Zn(OAc)_2$ in MeOH (5 mL) was added. The mixture was stirred in darkness for 18 h. The mixture was plug filtered (SiO_2, 6.5 cm x 4.5 cm; CH_2Cl_2), and concentrated. The crude product was adsorbed on silica and purified by dry loading into a 25G Redisep cartridge for automated column chromatography (SiO_2; CH_2Cl_2/Hex (0/100 – 50/50)). The product was precipitated from CH_2Cl_2 with MeOH to give a pink-colored solid in 72% (48 mg, 71 µmol) yield.

R_f (SiO_2; 1:1 CH_2Cl_2:Hex): 0.21.

Mp [ºC]: > 400, lit[5] 497.3 ± 0.5.

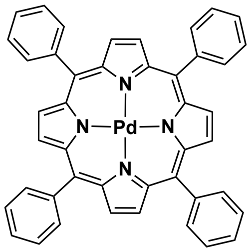
^{1}H NMR (300 MHz, $CDCl_3$, rt): δ [ppm] = 8.95 (s, 8H, **g**), 8.22 (d, ^3J = 7.7 Hz, 8H, **c**), 7.71 – 7.79 (m, 12H, **a,b**).

MS (MALDI-TOF, DCTB): *m/z (rel. Int.)* = 676.222 $[M]^{+\bullet}$ (100%).

IR (ATR): υ_{max} [cm^{-1}]: 3568, 1593, 1439, 1338, 1173, 1065, 992, 796, 702, 659.

UV/Vis (CH_2Cl_2, rt): λ [nm] (ε [M^{-1}cm^{-1}]) = 419 (468000), 547 (24000).

4.2.7 5,10,15,20-Tetraphenylporphyrinato palladium(II) (**PdTPP**)



PdTPP
$C_{44}H_{30}N_4Pd$
719.16 g/mol

A 50 mL two-necked round bottom flask equipped with a magnetic stir bar and a reflux condenser was charged with 10 equiv. $PdCl_2$ (289 mg, 1.63 mmol), dissolved in benzonitrile (25 mL) under argon and brought to reflux at 190 °C for 30 min. Tetraphenylporphyrin (**TPP**) (100 mg, 163 µmol) was added as solid under argon and the mixture was stirred at reflux in darkness for 6 h. The solvent was distilled off, the mixture was plug filtered (SiO_2, 6 cm x 3 cm; toluene), concentrated, and precipitated from toluene with MeOH. The solid was filtered, washed with MeOH and dried in vacuum, to give the product as red solid in 70% (82 mg, 114 µmol) yield.

R_f (SiO_2; 1:1 CH_2Cl_2:Hex): 0.61.

Mp [ºC]: 362.5 ± 3.6 (decomposition), lit[7] > 330.

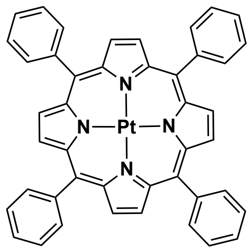
^{1}H NMR (300 MHz, $CDCl_3$, rt): δ [ppm] = 8.81 (s, 8H, **g**), 8.23 (d, ^3J = 7.7 Hz, 8H, **c**), 7.71 – 7.79 (m, 12H, **a,b**).

MS (MALDI-TOF, DCTB): *m/z (rel. int.)* = 718.280 $[M]^{+\bullet}$ (100%).

IR (ATR): υ_{max} [cm^{-1}]: 1595, 1440, 1351, 1175, 1072, 1012, 798, 750, 694.

UV/Vis (CH_2Cl_2, rt): λ [nm] (ε [M^{-1}cm^{-1}]) =415 (196000), 522 (26000), 555 (2600).

4.2.8 5,10,15,20-Tetraphenylporphyrinato platinum(II) (**PtTPP**)



PtTPP
$C_{44}H_{28}N_4Pt$
807.82 g/mol

A 50 mL two-necked round bottom flask equipped with a magnetic stir bar and a reflux condenser was charged with 10 equiv. $Pt(acac)_2$ (641 mg, 1.63 mmol), dissolved in benzonitrile (25 mL) under argon and brought to reflux at 190 °C for 30 min. Tetraphenylporphyrin (**TPP**) (100 mg, 163 µmol) was added as solid under argon and the mixture was stirred at reflux in darkness for 6 h. The solvent was distilled off, the mixture was plug filtered (SiO_2, 6 cm x 3 cm; toluene), concentrated, and precipitated from toluene with MeOH. The solid was filtered, washed with MeOH and dried in vacuum, to give the product as red solid in 60% (80 mg, 97.8 µmol) yield.

R_f (SiO_2; 1:1 CH_2Cl_2:Hex): 0.54.

Mp [ºC]: 361.4 ± 1.0 (decomposition), lit[8] > 330.

^{1}H NMR (300 MHz, $CDCl_3$, rt): δ [ppm] = 8.75 (s, 8H, **g**), 8.10 (d, ^3J = 7.8 Hz, 8H, **c**), 7.72 – 7.78 (m, 12H, **a,b**).

MS (MALDI-TOF, DCTB): *m/z (rel. int.)* = 808.338 $[M]^{+\bullet}$ (100%).

IR (ATR): υ_{max} [cm^{-1}]: 1595, 1440, 1358, 1316, 1175, 1076, 1016, 837, 797, 751, 702.

UV/Vis (CH_2Cl_2, rt): λ [nm] (ε [$M^{-1}cm^{-1}$]) = 401 (230000), 509 (27000), 539 (5800) 595 (2500).

4.3 Spectral Appendix (NMR, MS, IR, UV/Vis, Mp)

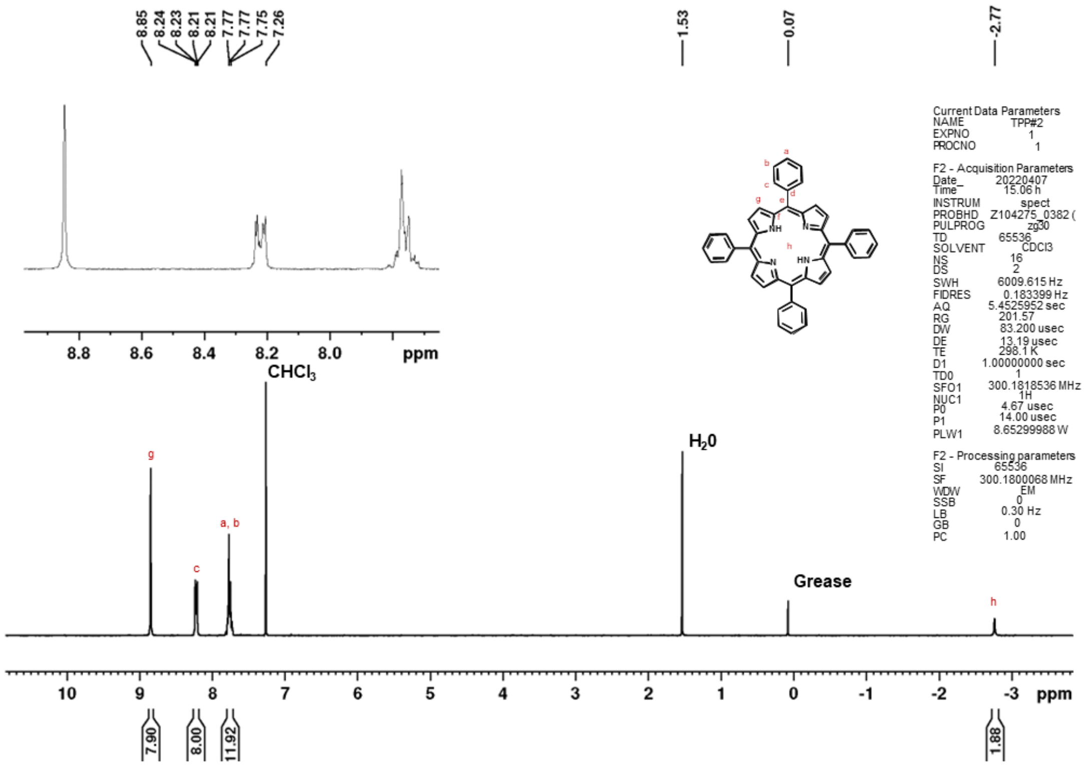


Figure S10. ^1H NMR (300 MHz, $CDCl_3$, rt) of **TPP**.

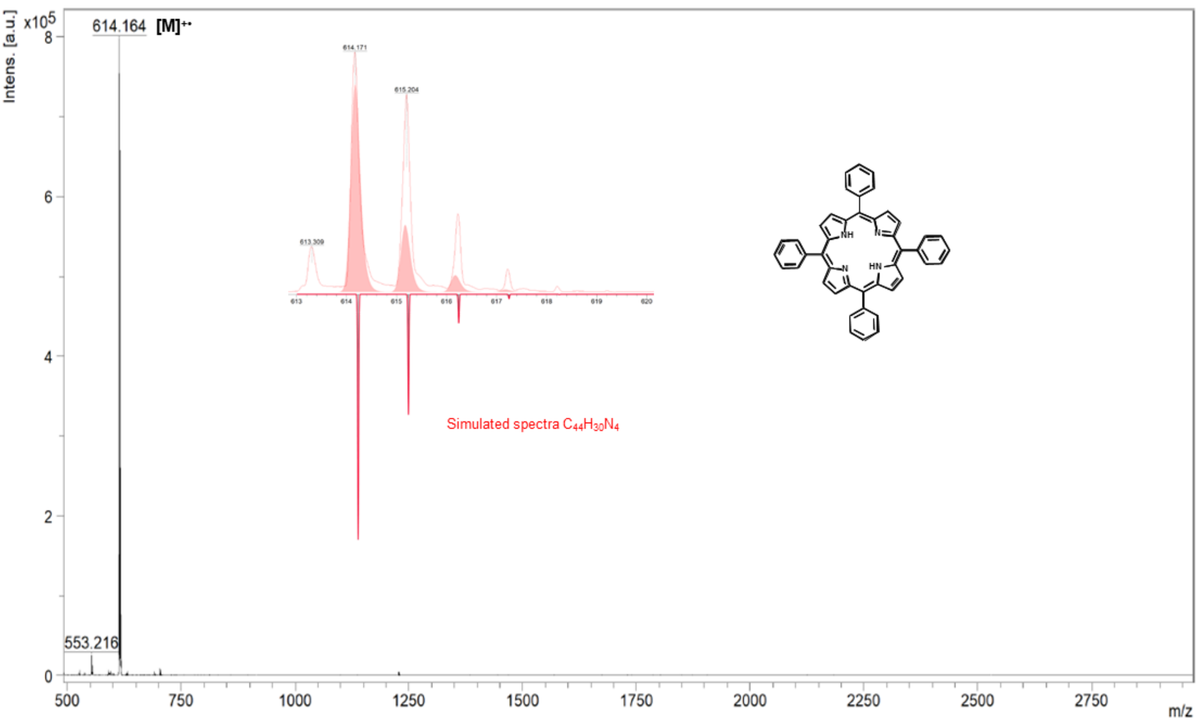


Figure S11. MS (MALDI-TOF, DCTB) of **TPP**.

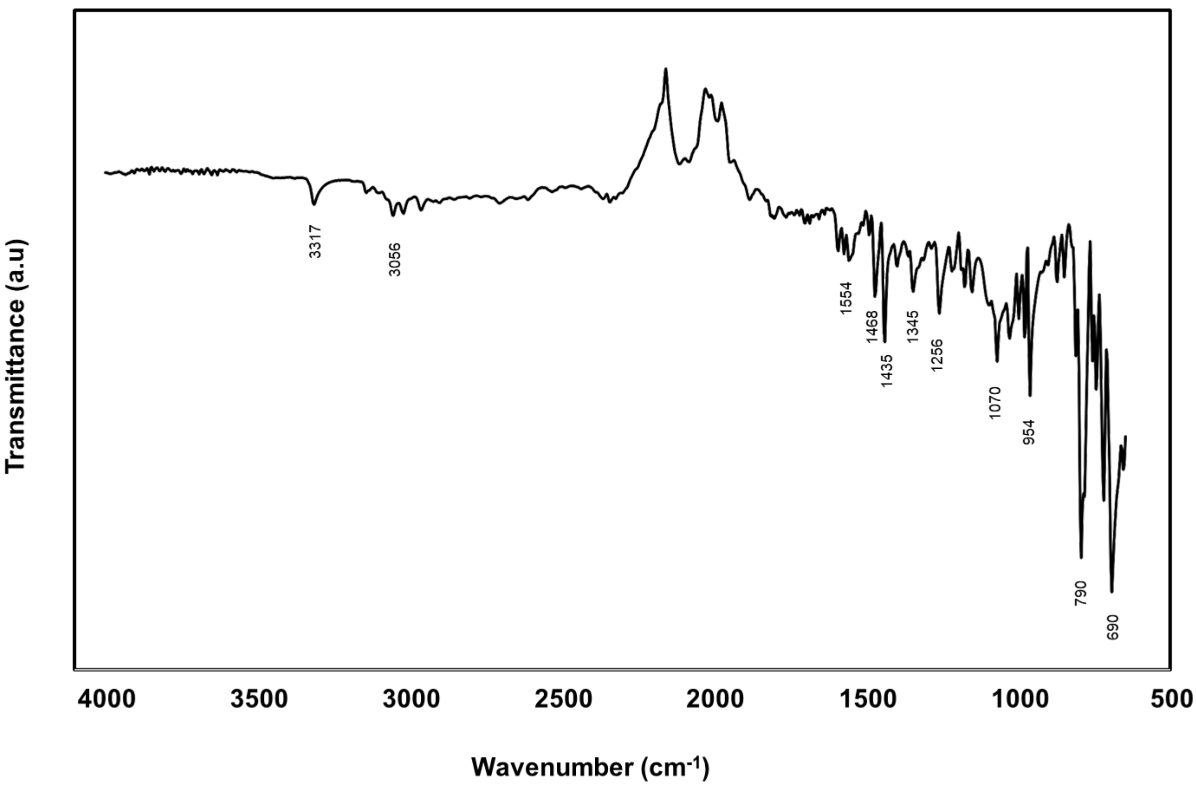


Figure S12. IR (ATR) of **TPP**.

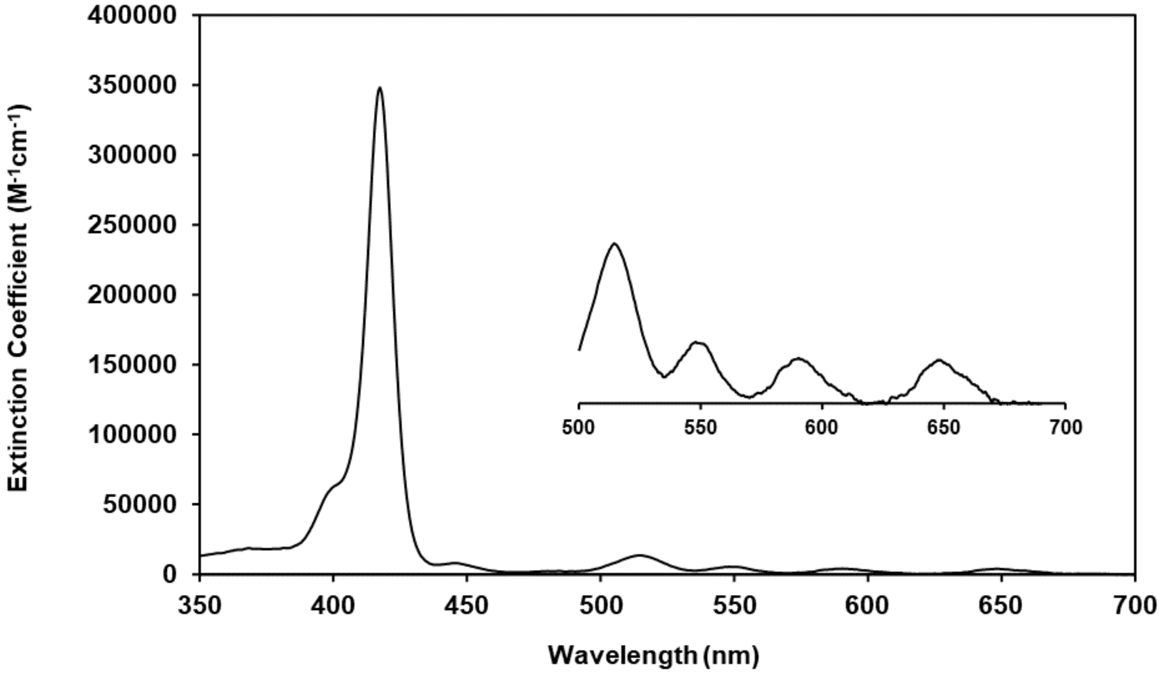


Figure S13. UV/Vis (CH_2Cl_2, rt) for **CuTPP**.

Method	TPP
Start temperature:	350 °C
Temperature gradient	1.0 °C/min
Melting result:	acc. EU pharmacopoeia
Sample ID:	TPP

Automatic:

Left	Center	Right

Average:

Standard deviation:

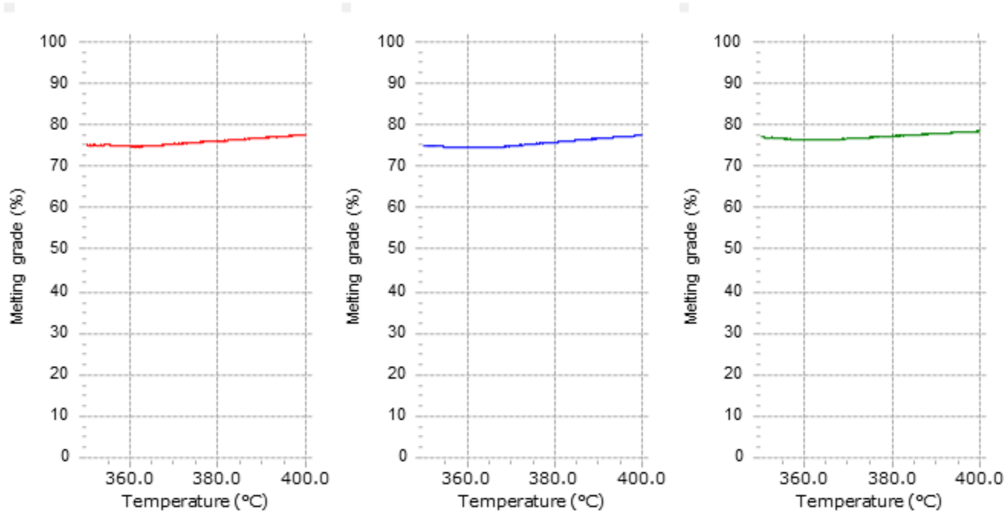


Figure S14. Melting point measurement of **TPP**.

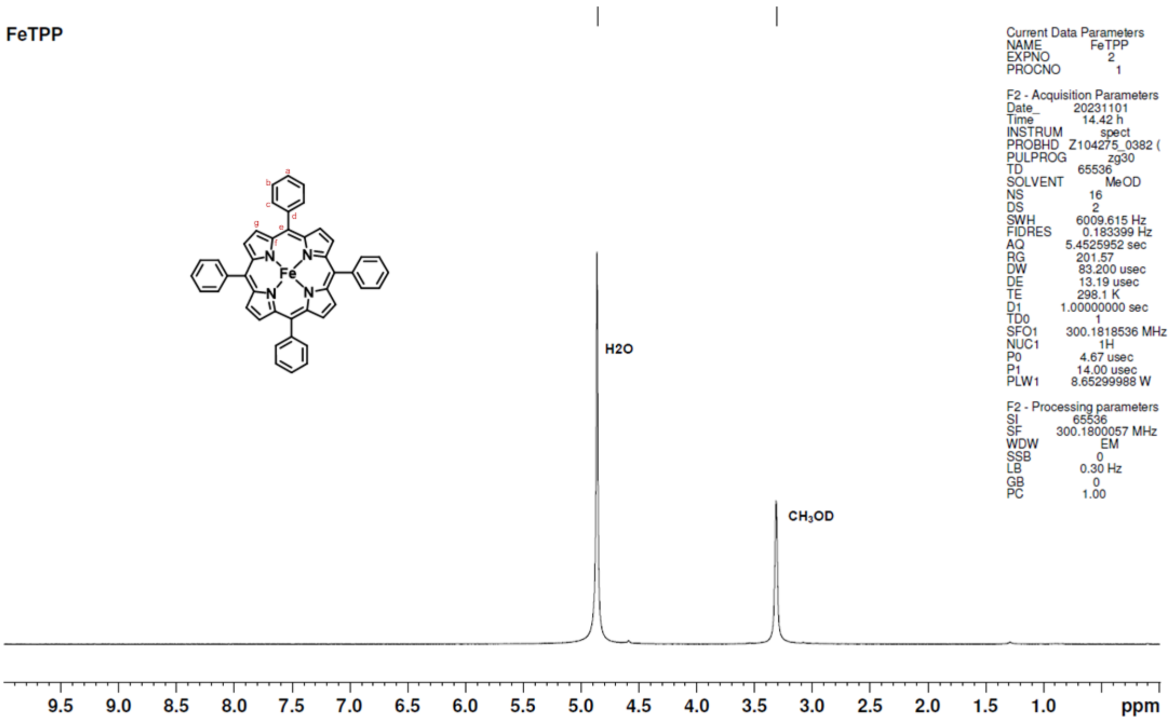


Figure S15. ^{1}H NMR (300 MHz, CD_3OD, rt) of **FeTPP**.

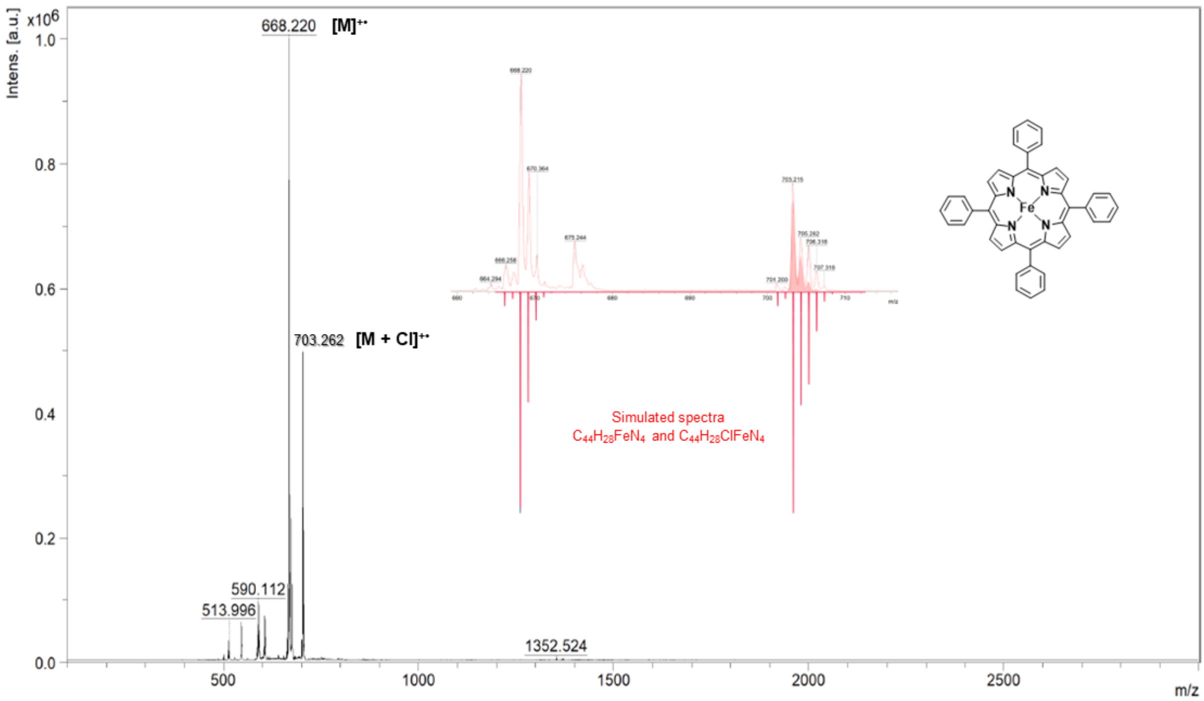


Figure S16. MS (MALDI-TOF, DCTB) of **FeTPP**.

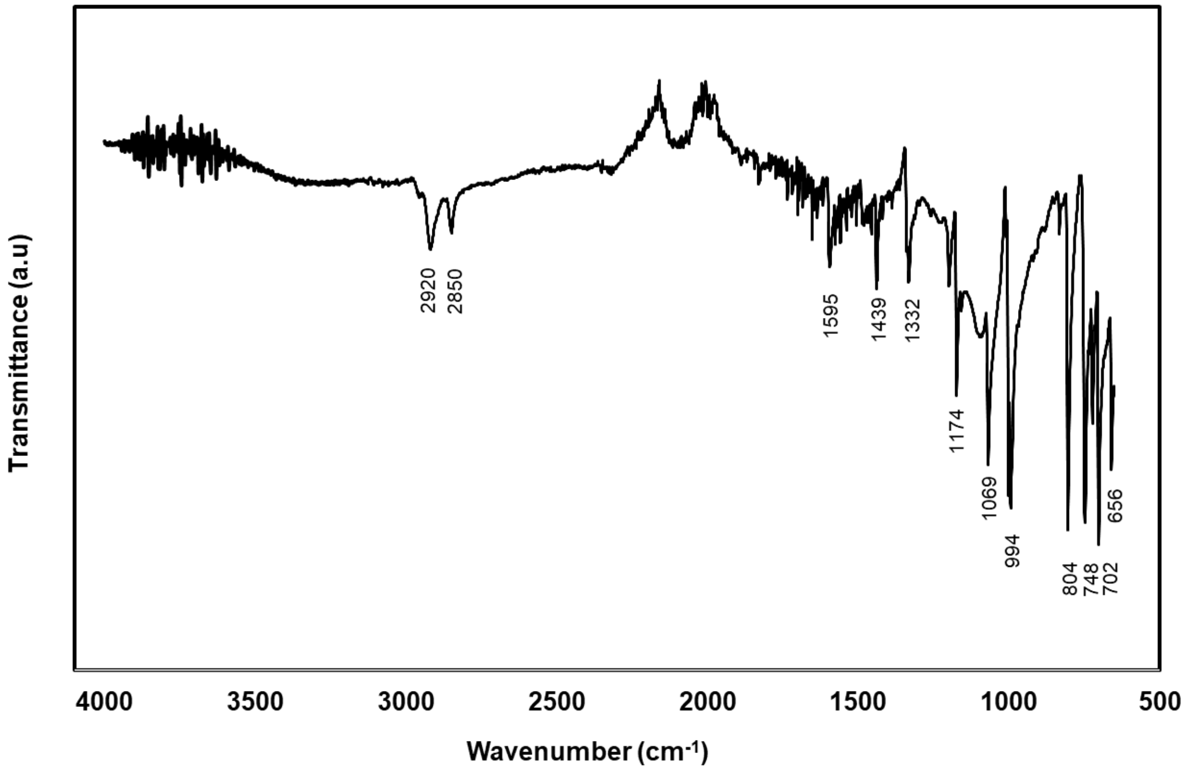


Figure S17. IR (ATR) of **FeTPP**.

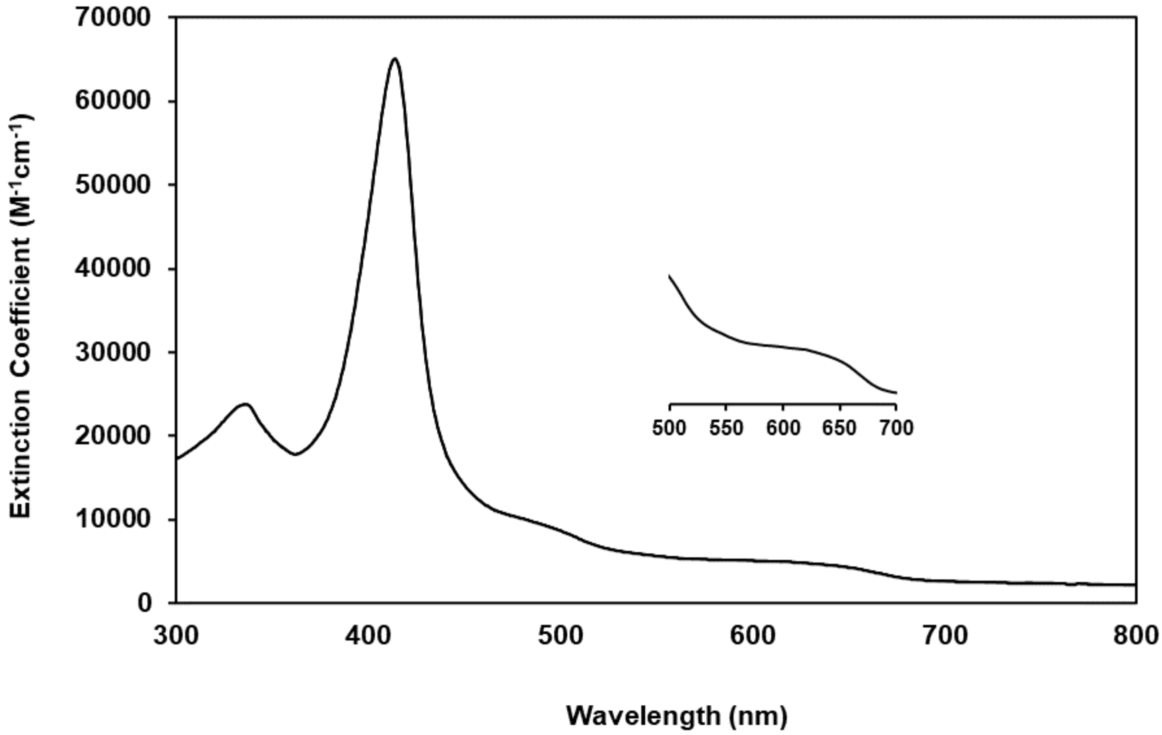


Figure S18. UV/Vis (MeOH, rt) for **FeTPP**.

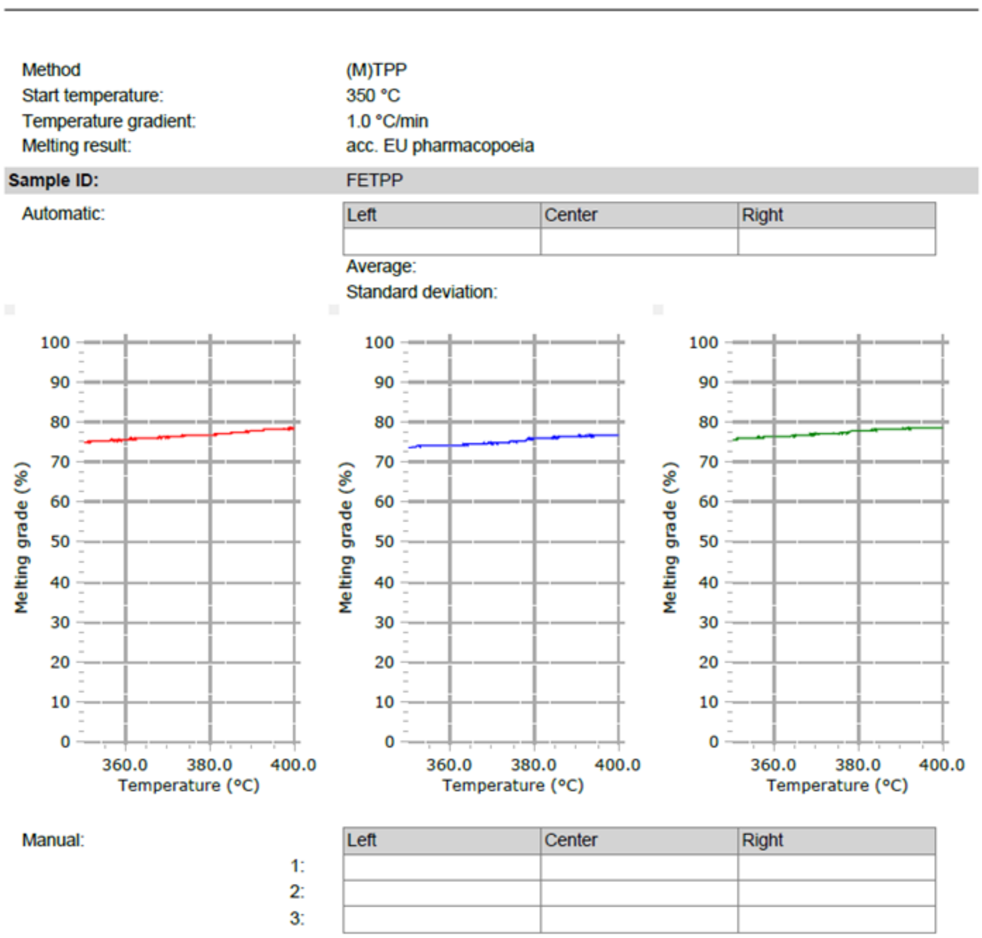


Figure S19. Melting point measurement of **FeTPP**.

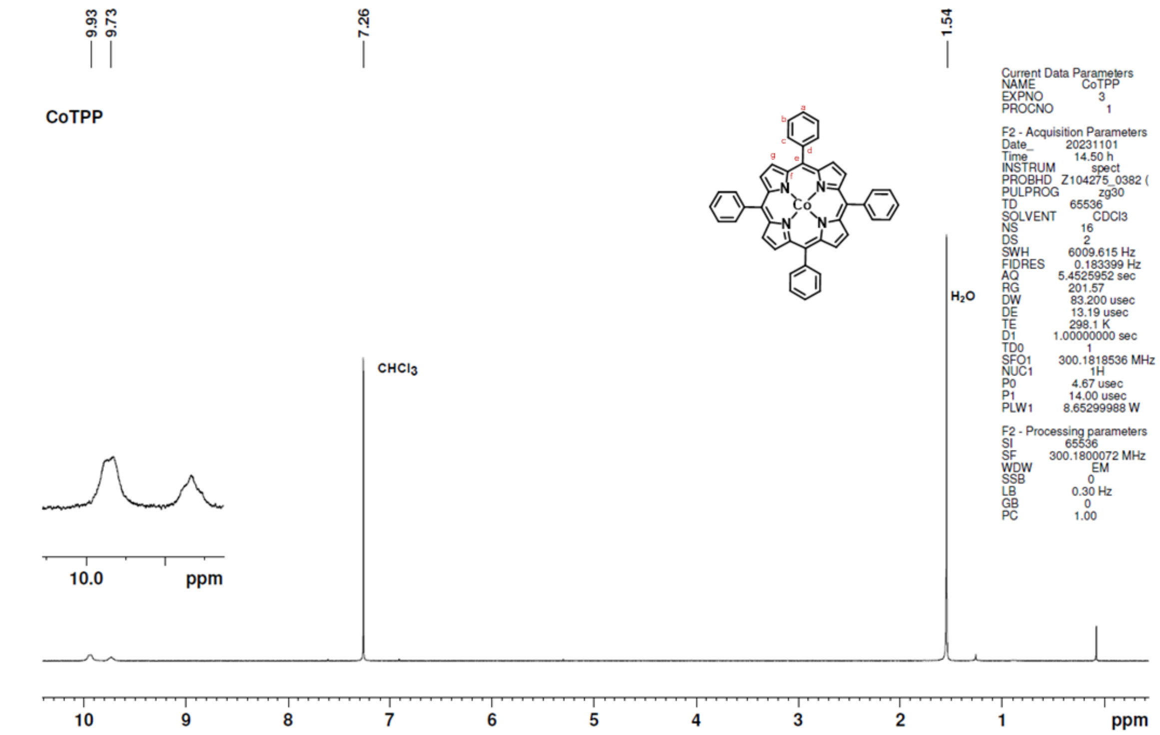


Figure S20. [1]H NMR (300 MHz, $CDCl_3$, rt) of **CoTPP**.

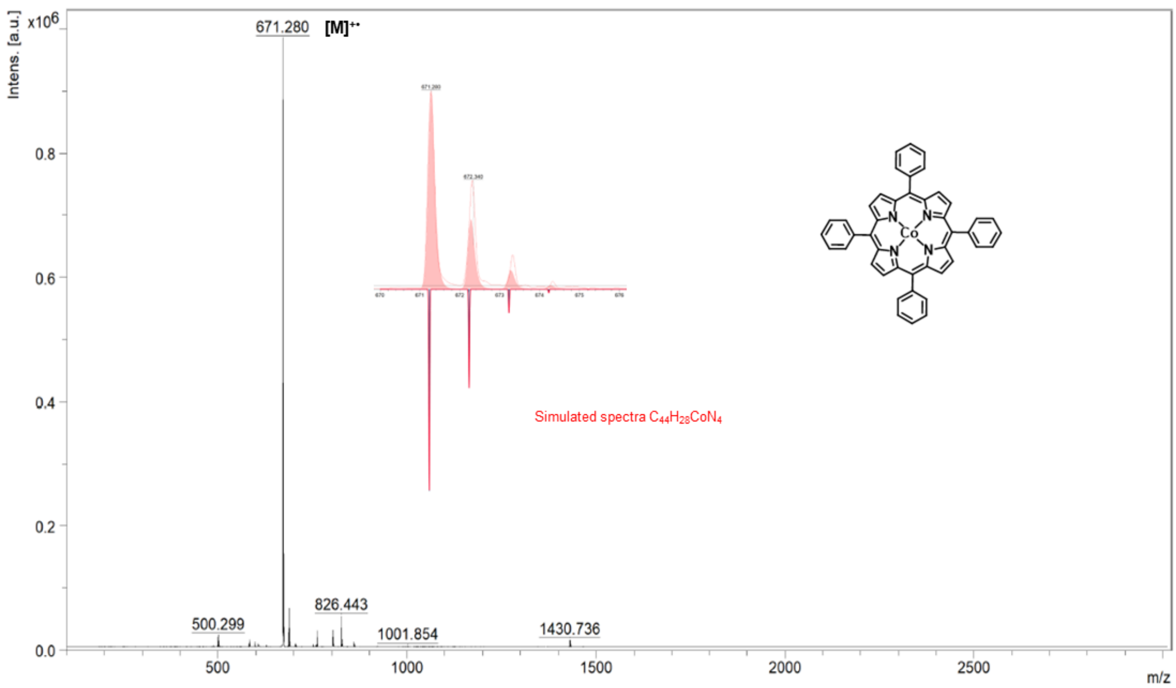


Figure S21. MS (MALDI-TOF, DCTB) of **CoTPP**.

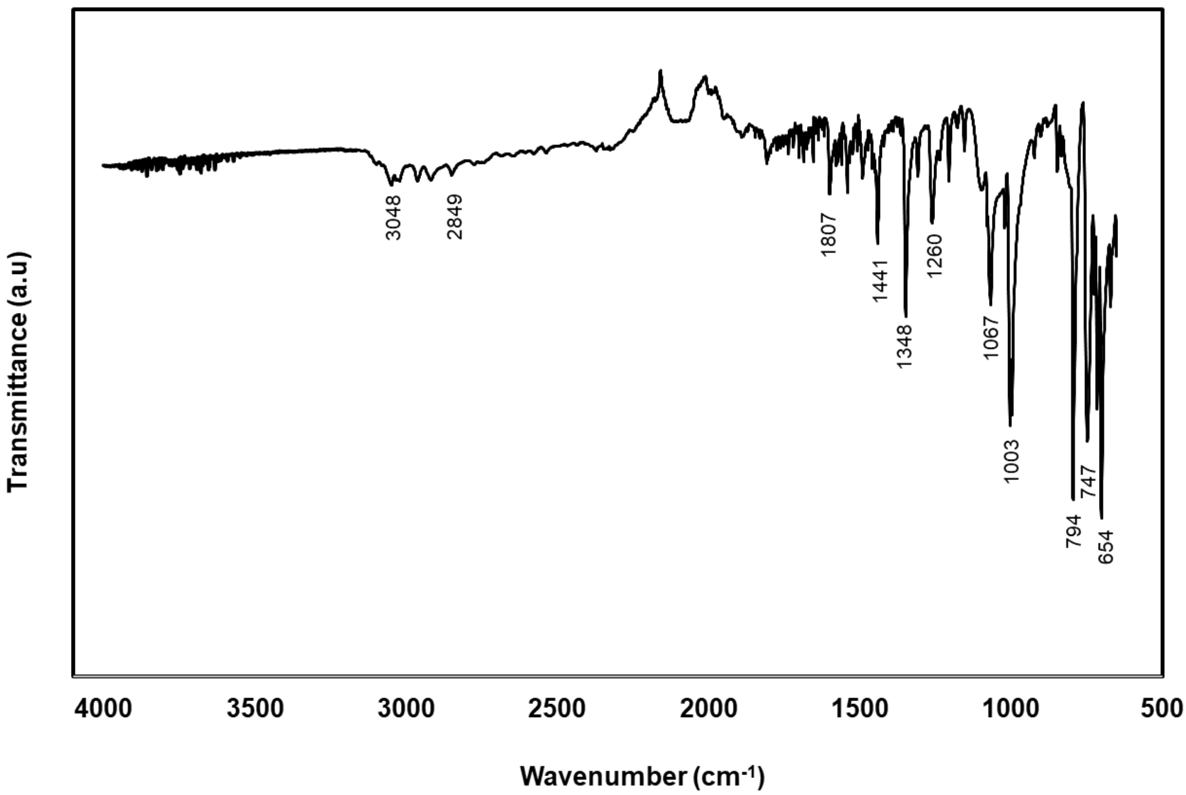


Figure S22. IR (ATR) of **CoTPP**.

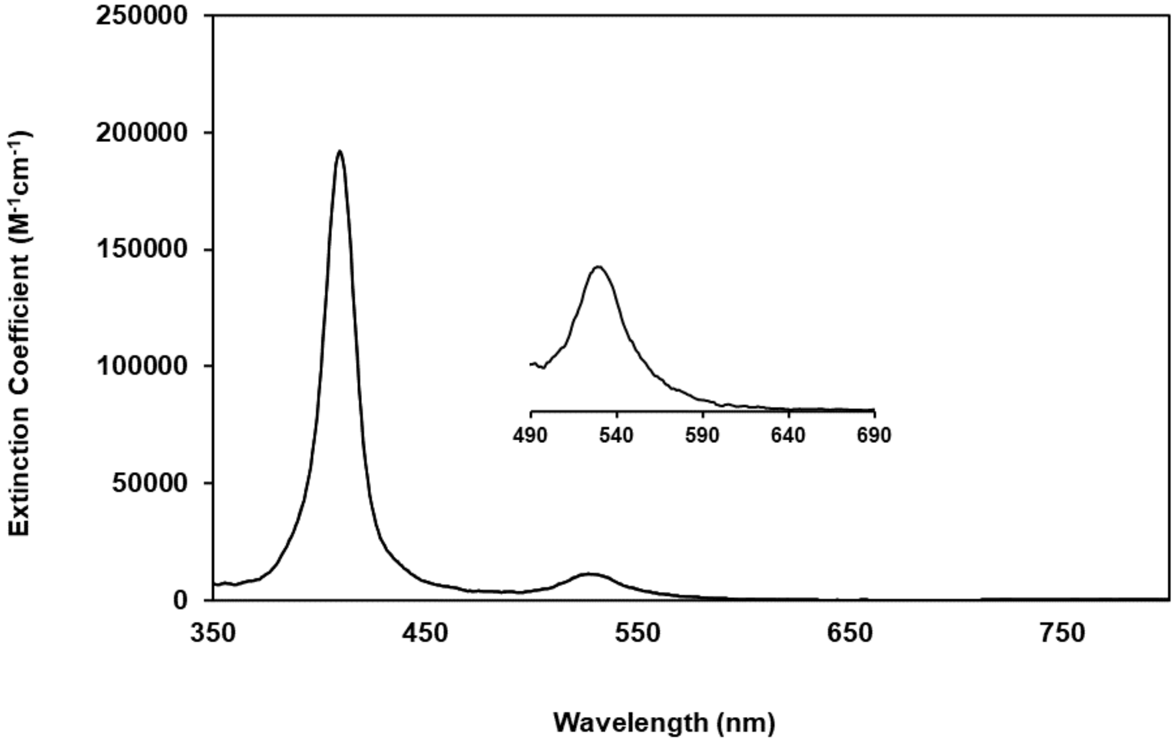


Figure S23. UV/Vis (CH_2Cl_2, rt) for **CoTPP**.

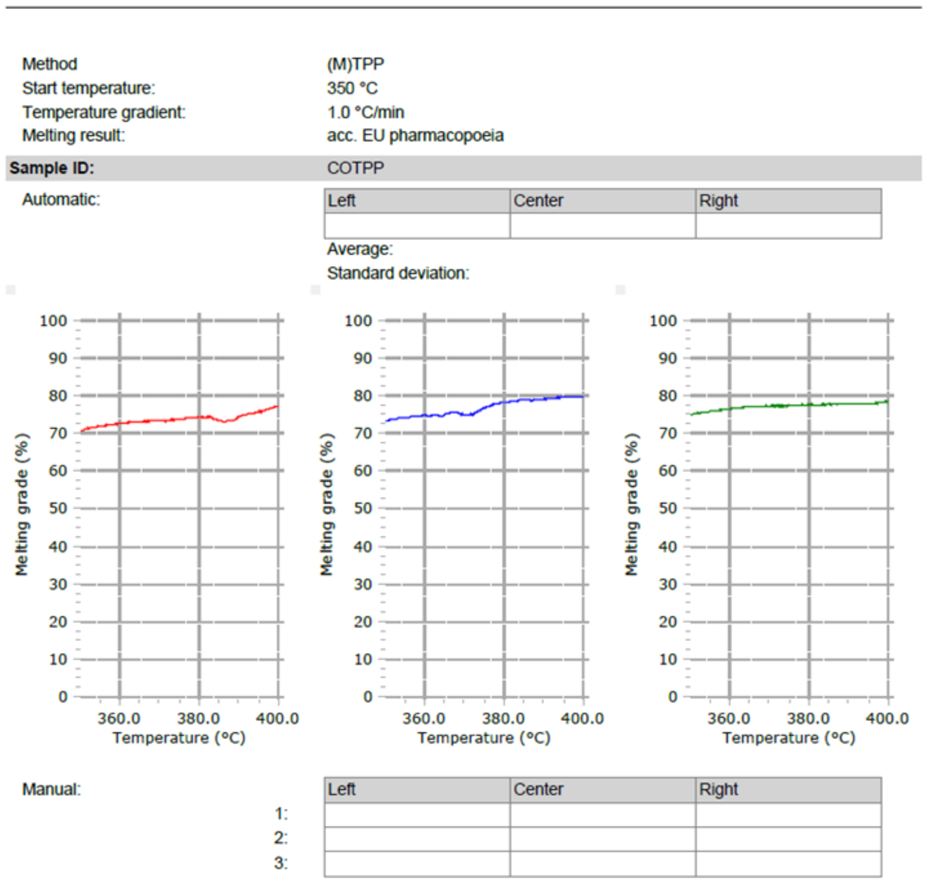


Figure S24. Melting point measurement of **CoTPP**.

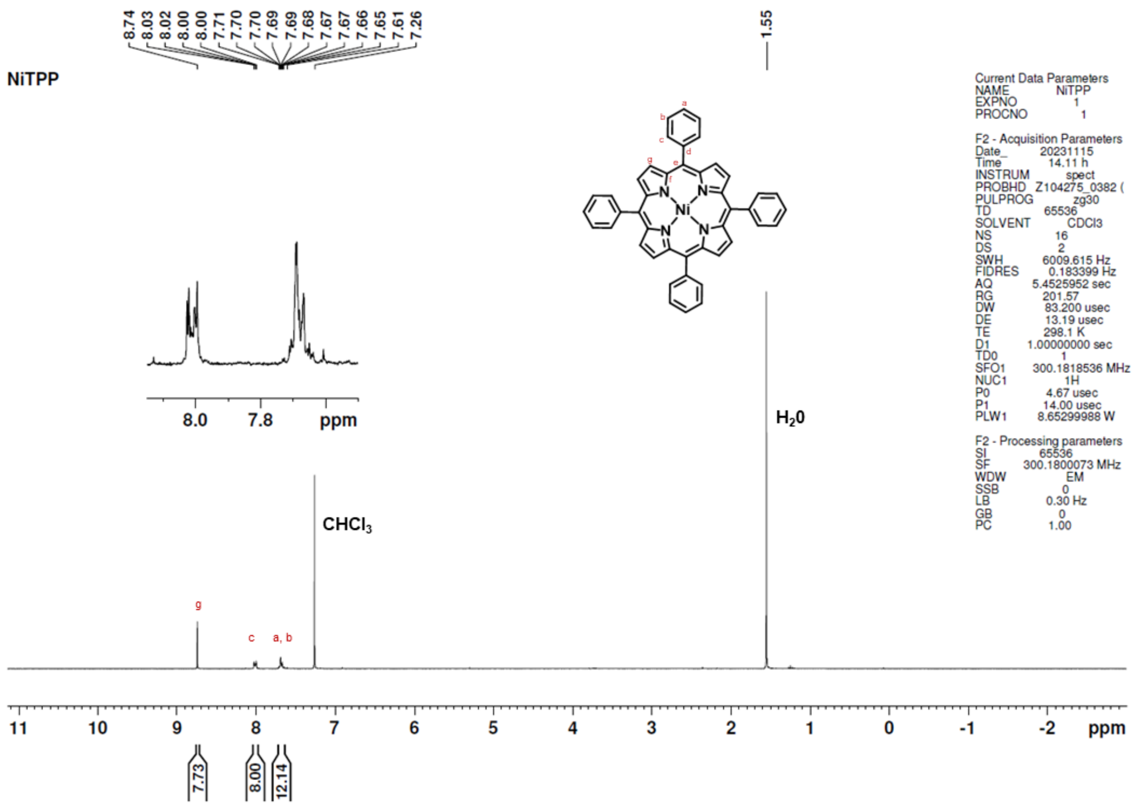


Figure S25. ^{1}H NMR (300 MHz, $CDCl_3$, rt) of **NiTPP**.

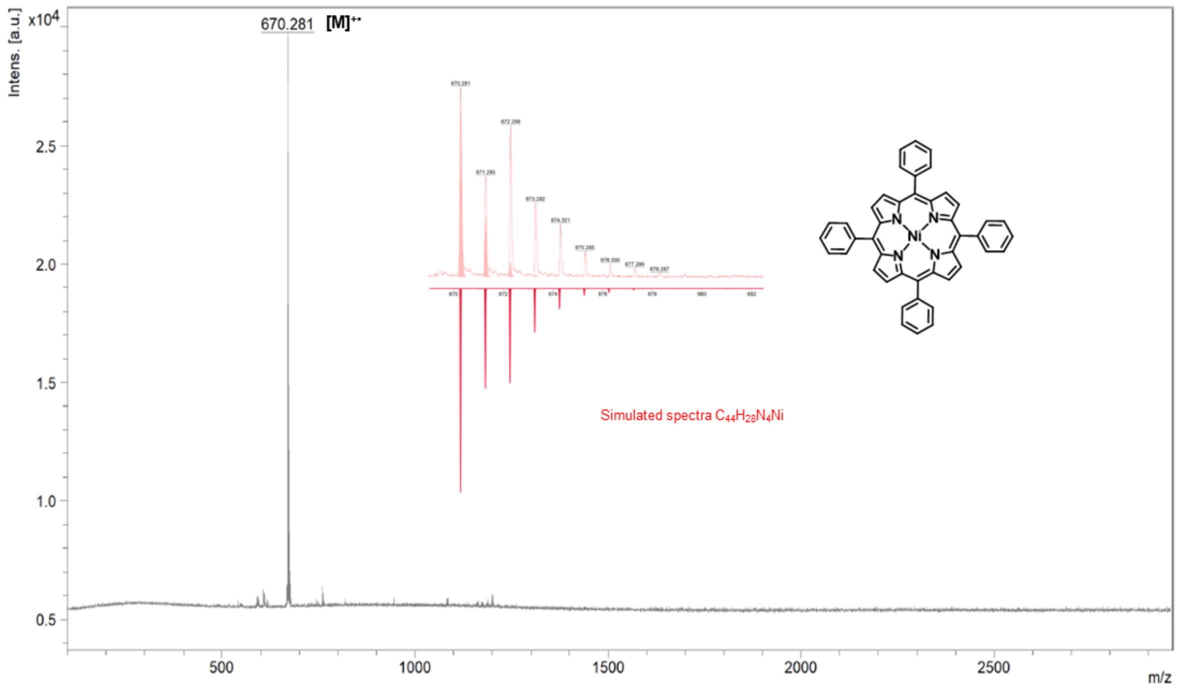


Figure S26. MS (MALDI-TOF, DCTB) of **NiTPP**.

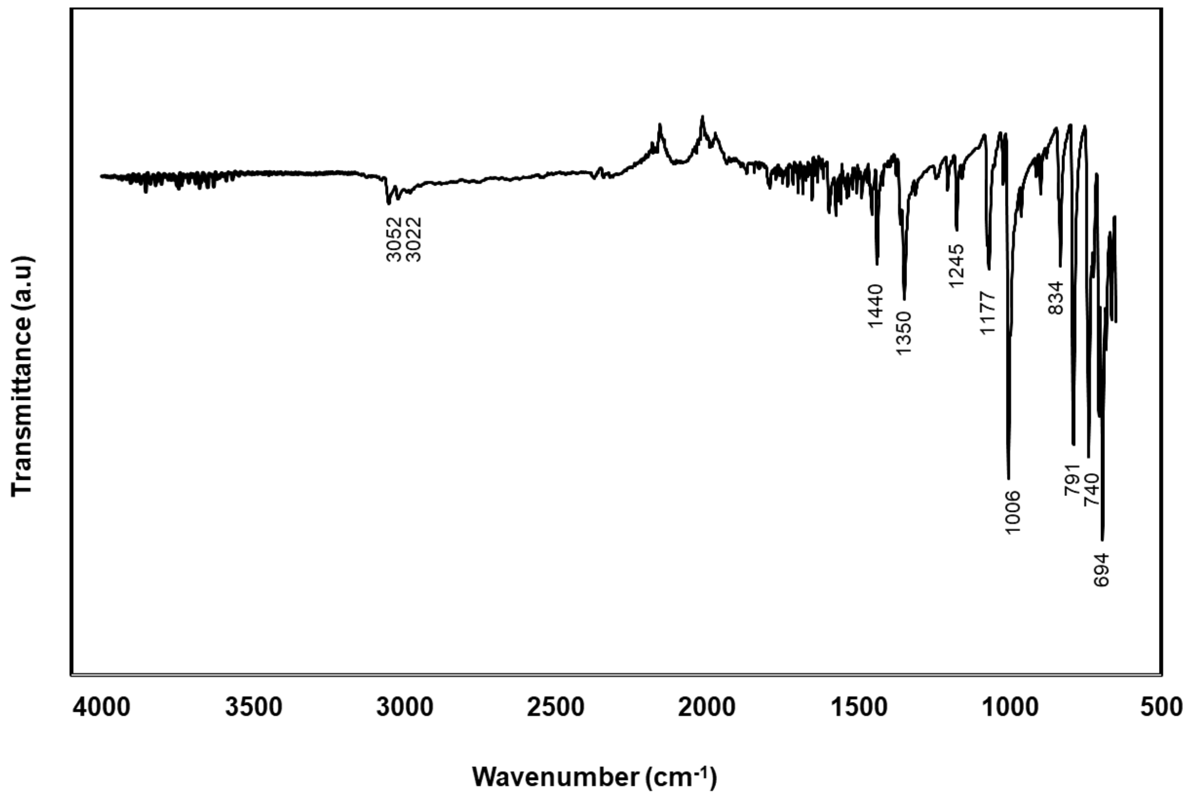


Figure S27. IR (ATR) of **NiTPP**.

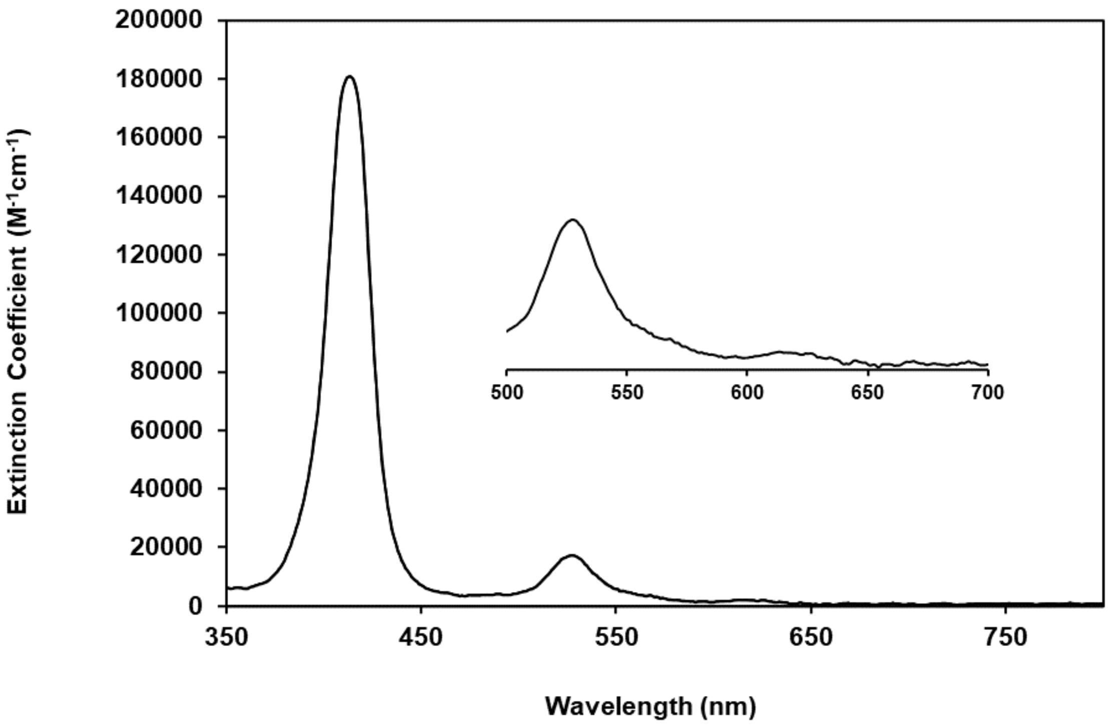
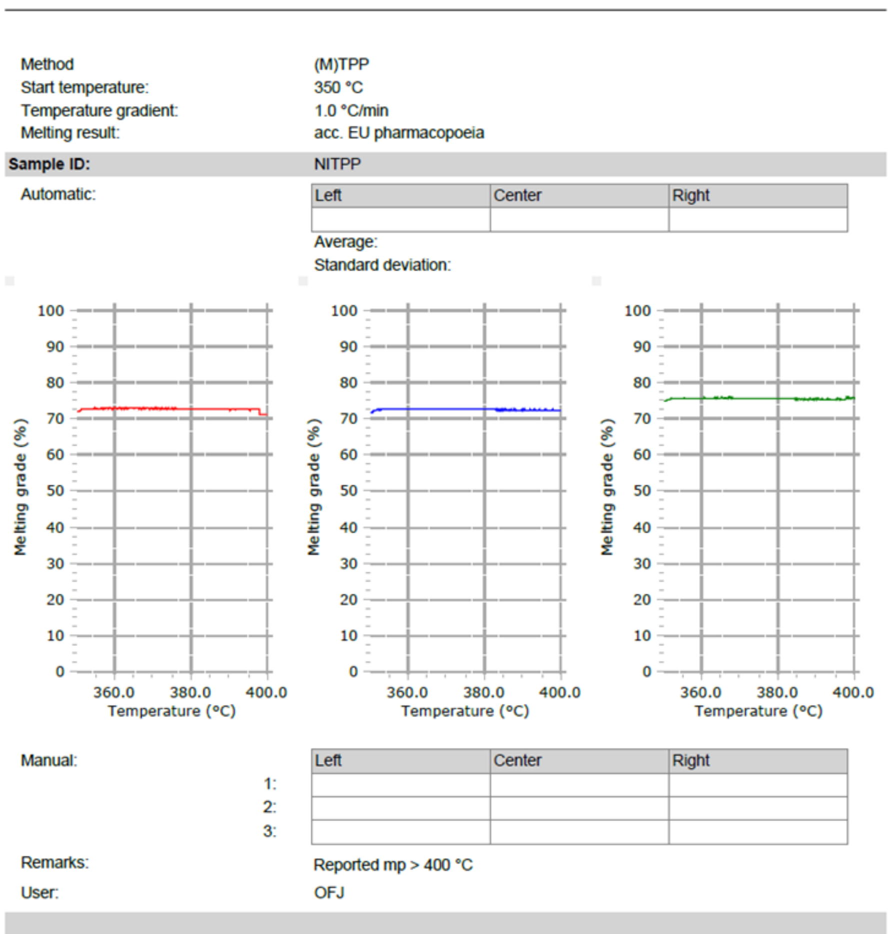


Figure S28. UV/Vis (CH_2Cl_2, rt) for **NiTPP**.


Method: (M)TPP
Start temperature: 350 °C
Temperature gradient: 1.0 °C/min
Melting result: acc. EU pharmacopoeia

Sample ID: NITPP

Automatic:

Left	Center	Right

Average:
Standard deviation:

Manual:

	Left	Center	Right
1:			
2:			
3:			

Remarks: Reported mp > 400 °C
User: OFJ

Figure S29. Melting point measurement of **NiTPP**.

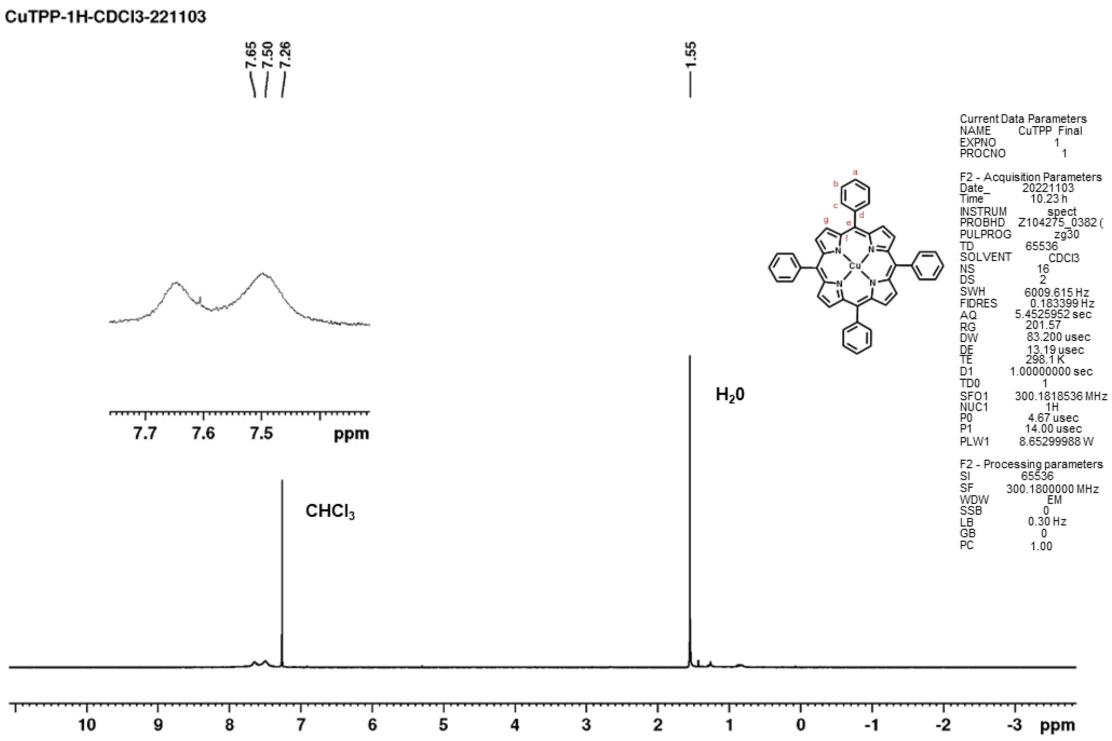


Figure S30. ^{1}H NMR (300 MHz, $CDCl_3$, rt) of **CuTPP**.

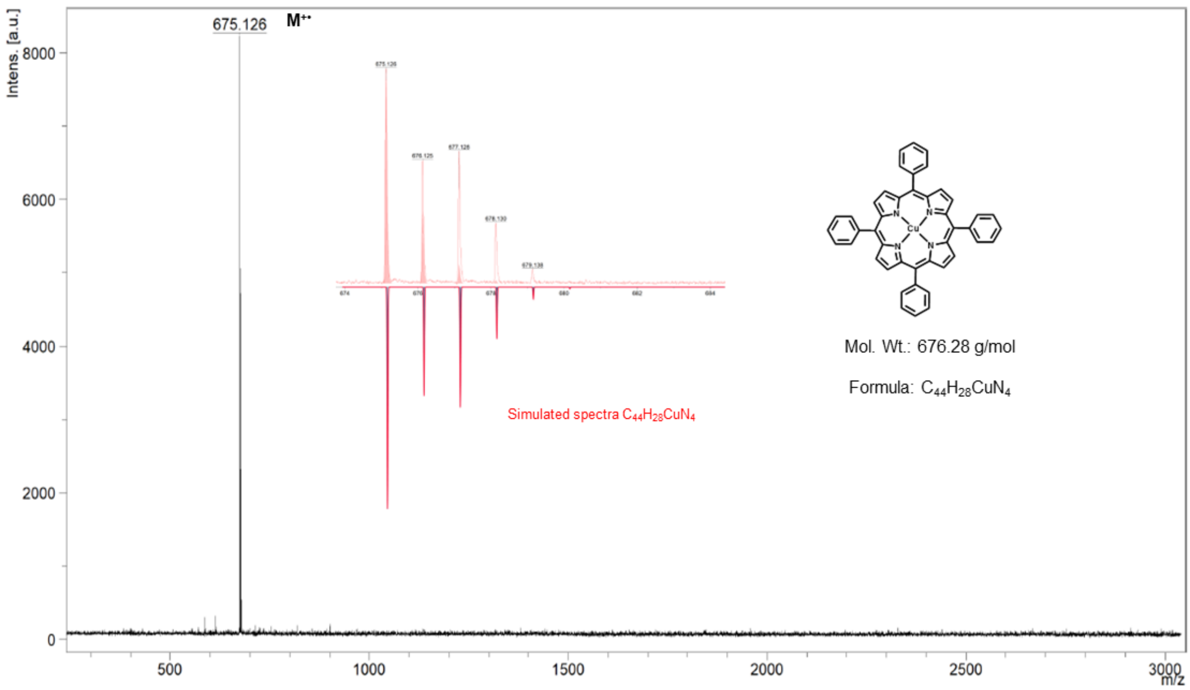


Figure S31. MS (MALDI-TOF, DCTB) of **CuTPP**.

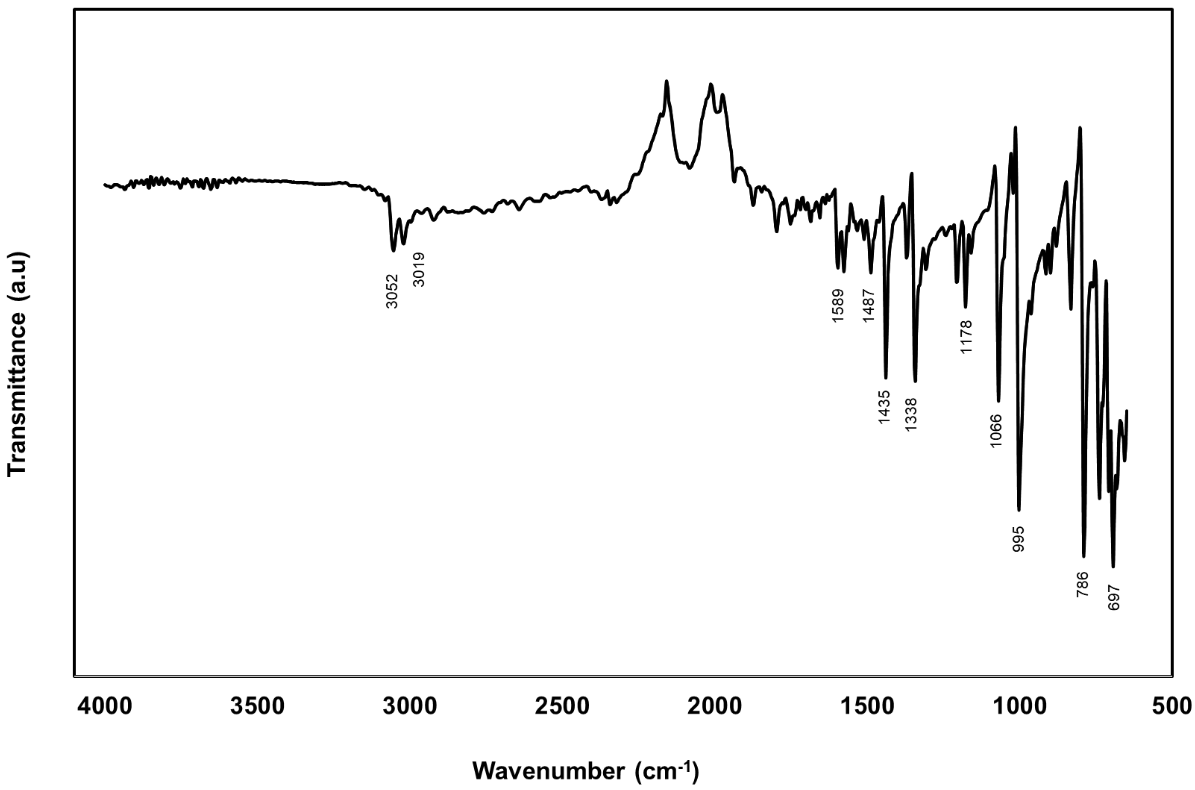


Figure S32. IR (ATR) of **CuTPP**.

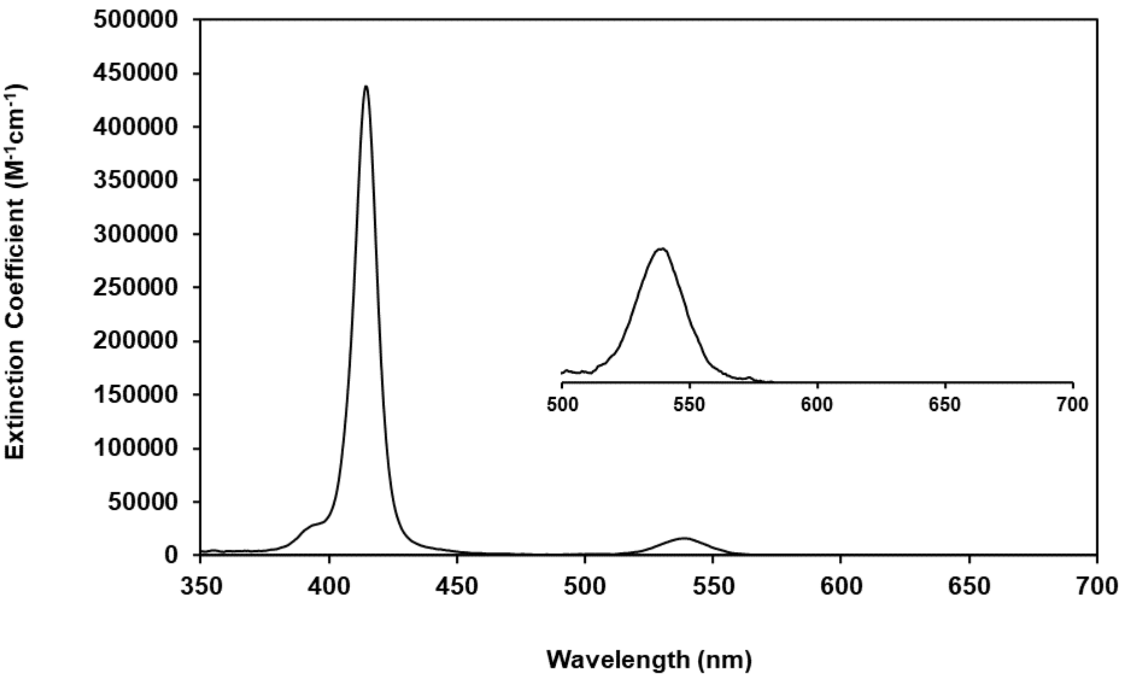
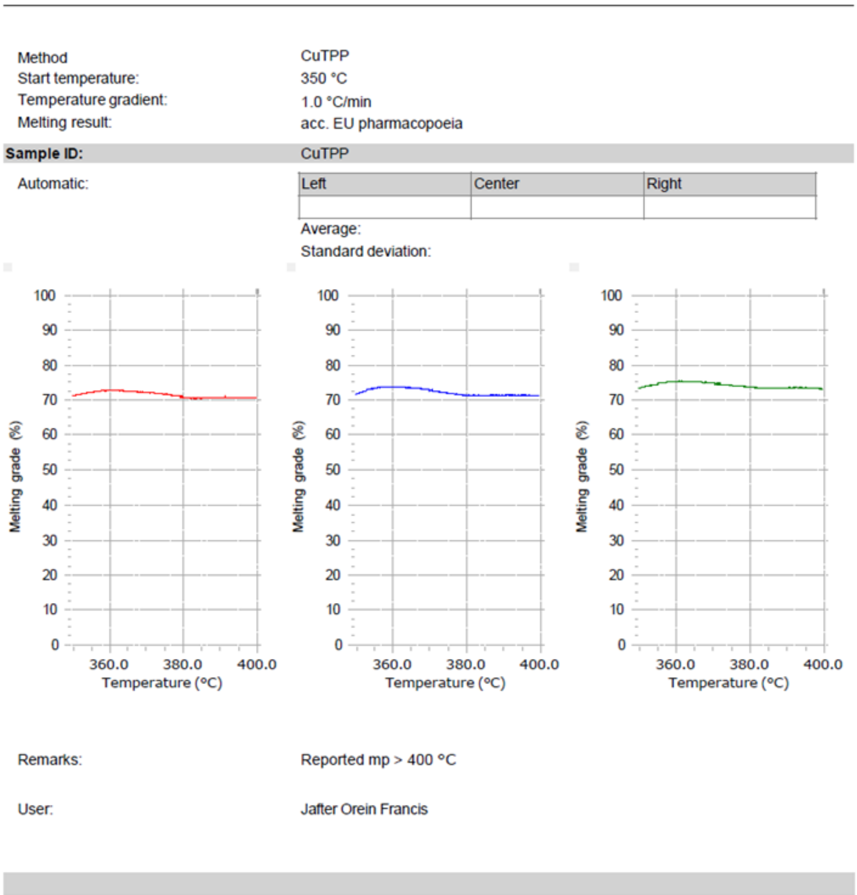


Figure S33. UV/Vis (CH_2Cl_2, rt) for **CuTPP**.



Method	CuTPP
Start temperature:	350 °C
Temperature gradient:	1.0 °C/min
Melting result:	acc. EU pharmacopoeia
Sample ID:	CuTPP

Automatic:

Left	Center	Right

Average:
Standard deviation:

Remarks: Reported mp > 400 °C

User: Jafter Orein Francis

Figure S34. Melting point measurement of **CuTPP**.

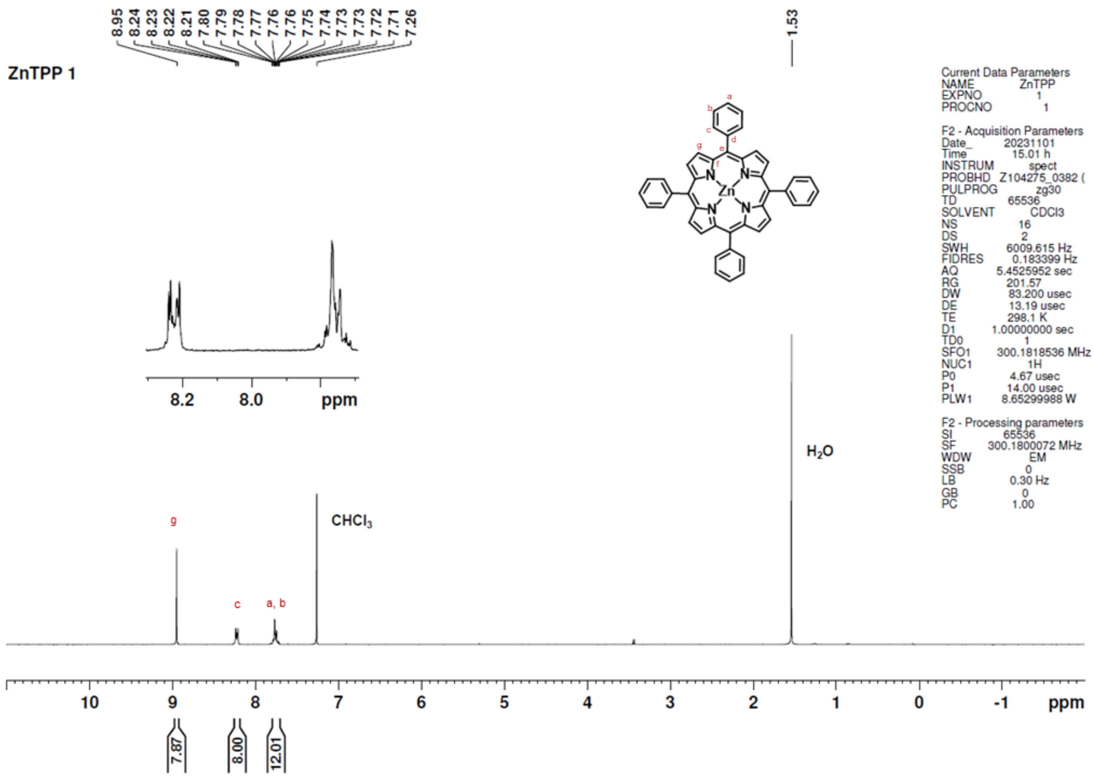


Figure S35. ^{1}H NMR (300 MHz, $CDCl_3$, rt) of **ZnTPP**.

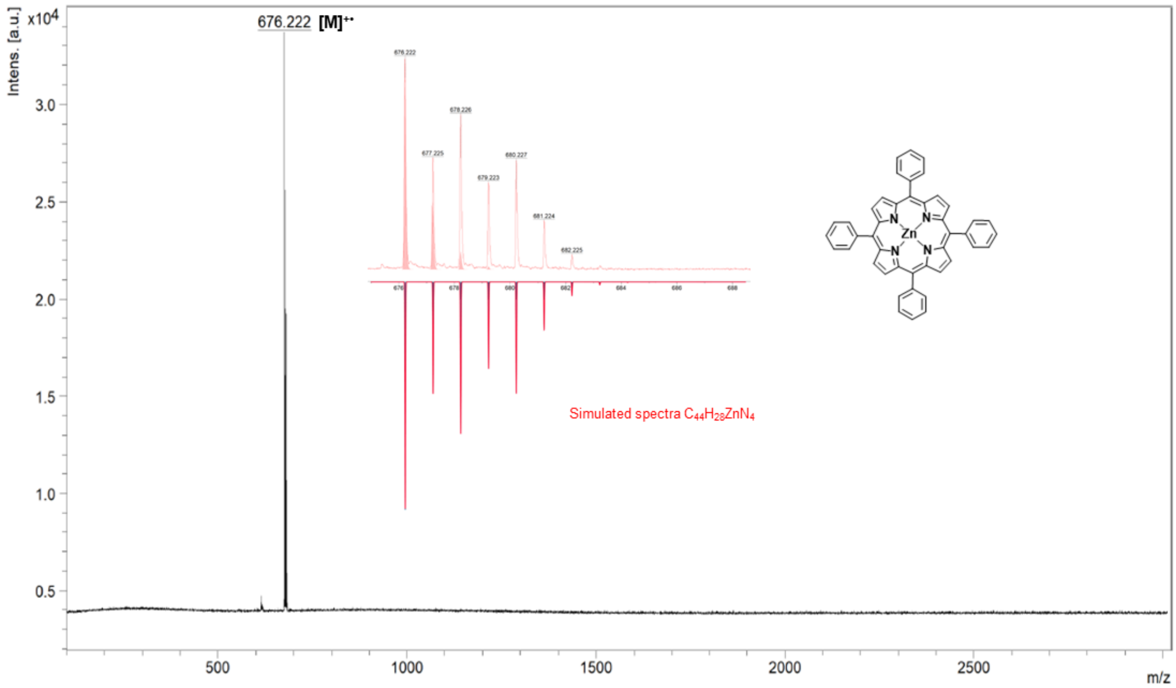


Figure S36. MS (MALDI-TOF, DCTB) of **ZnTPP**.

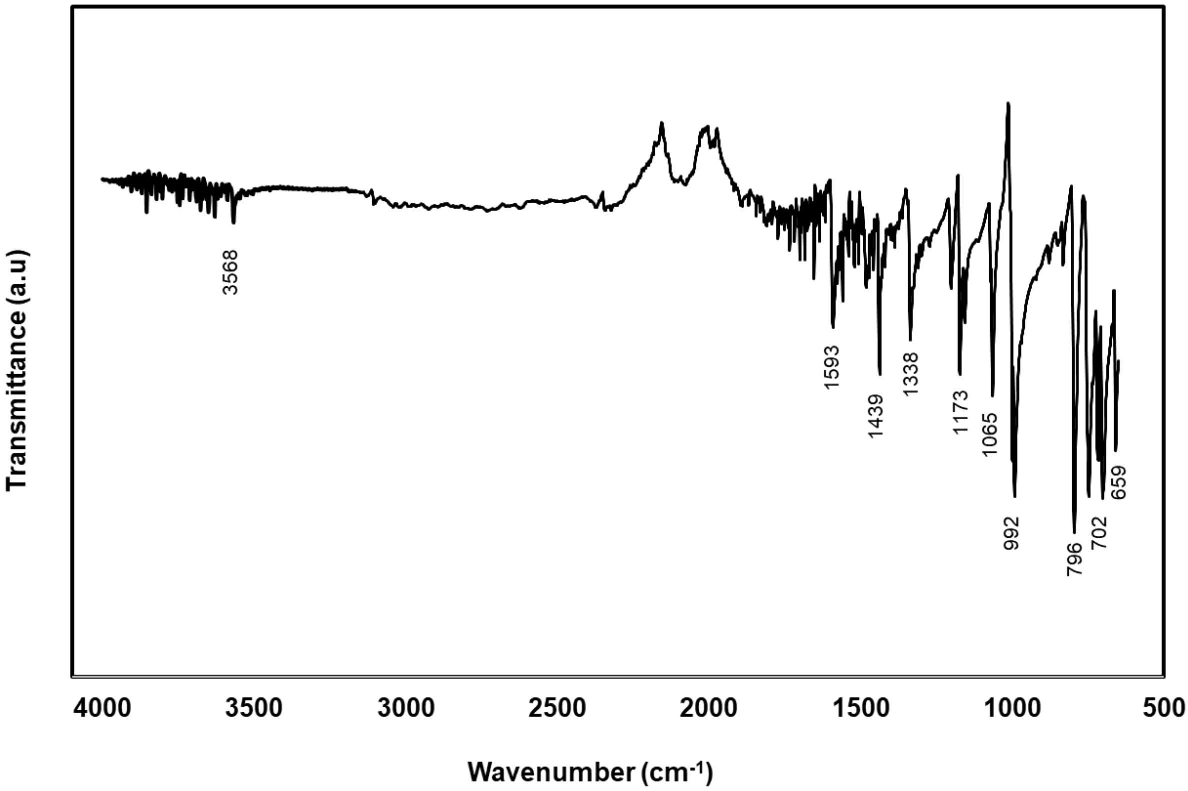


Figure S37. IR (ATR) of **ZnTPP**.

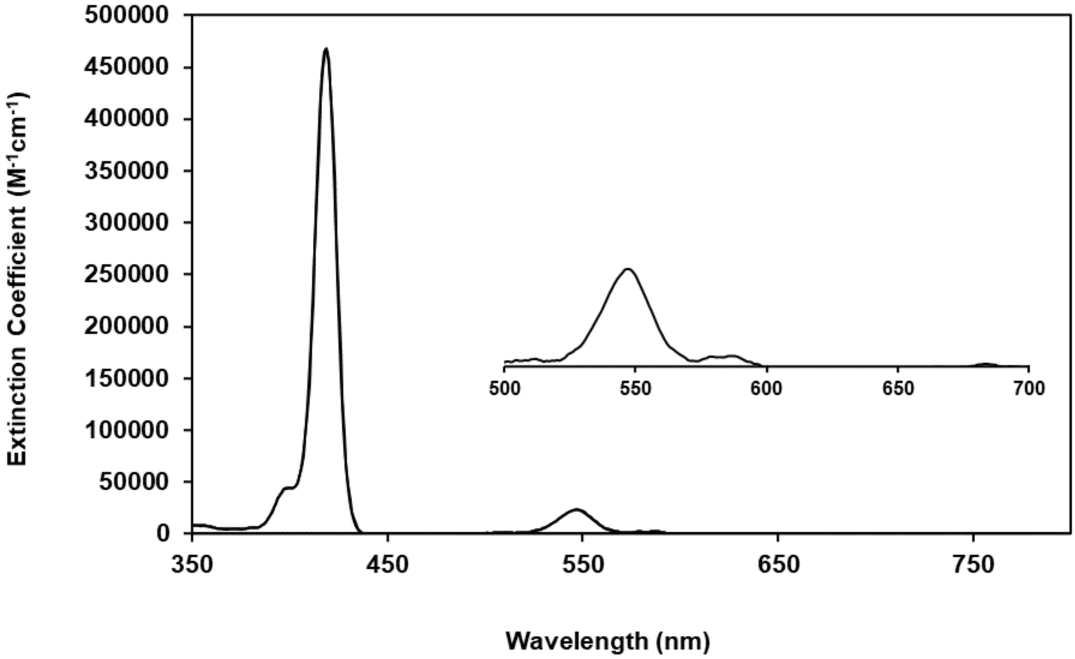


Figure S38. UV/Vis (CH_2Cl_2, rt) for **ZnTPP**.

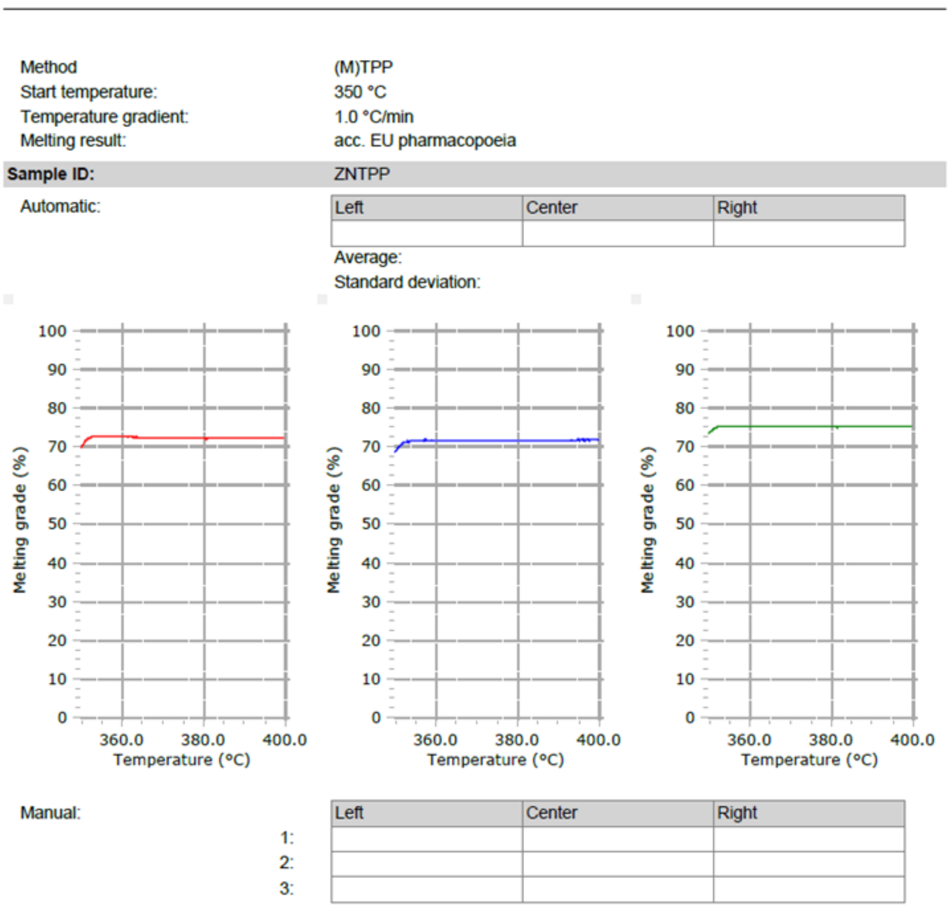


Figure S39. Melting point measurement of **ZnTPP**.

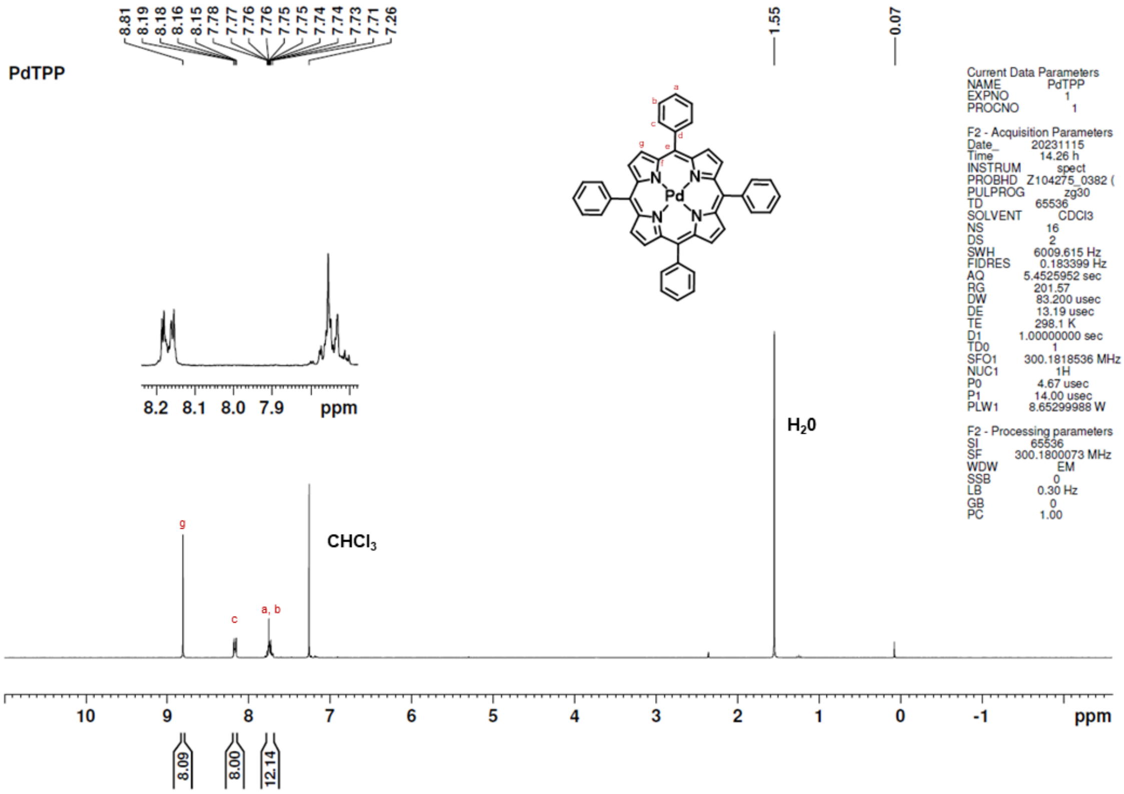


Figure S40. ^{1}H NMR (300 MHz, CDCl$_3$, rt) of **PdTPP**.

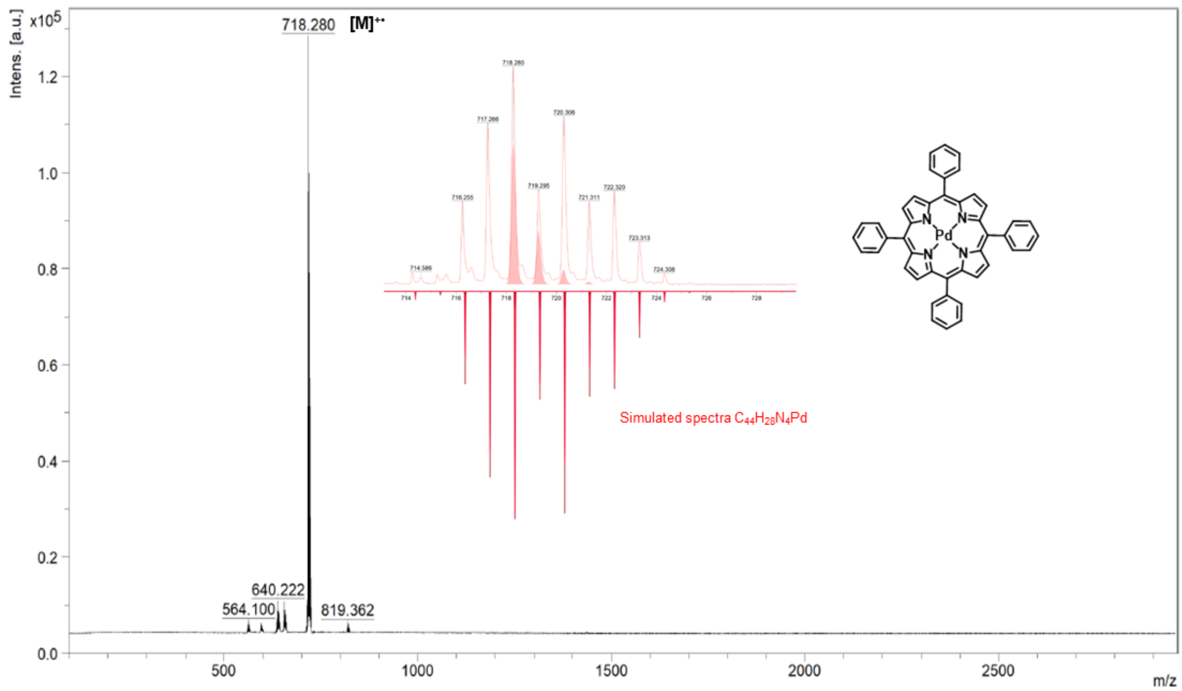


Figure S41. MS (MALDI-TOF, DCTB) of **PdTPP**.

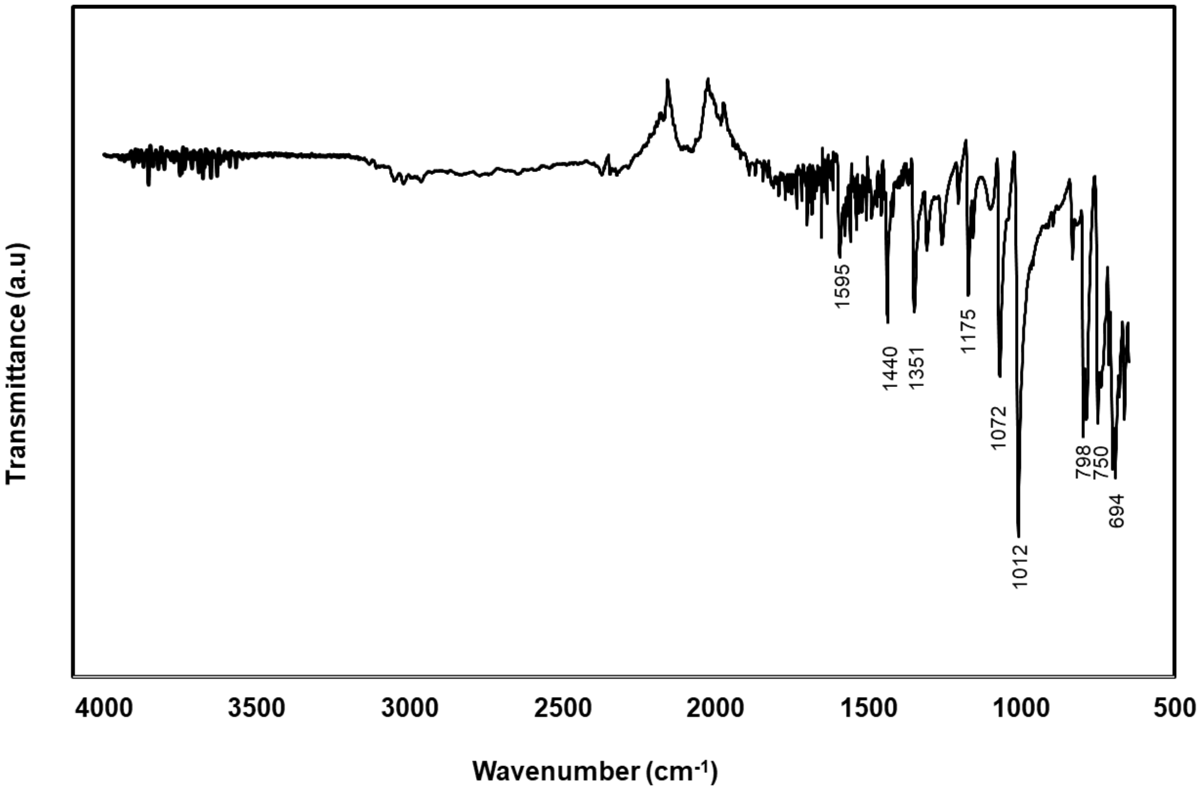


Figure S42. IR (ATR) of **PdTPP**.

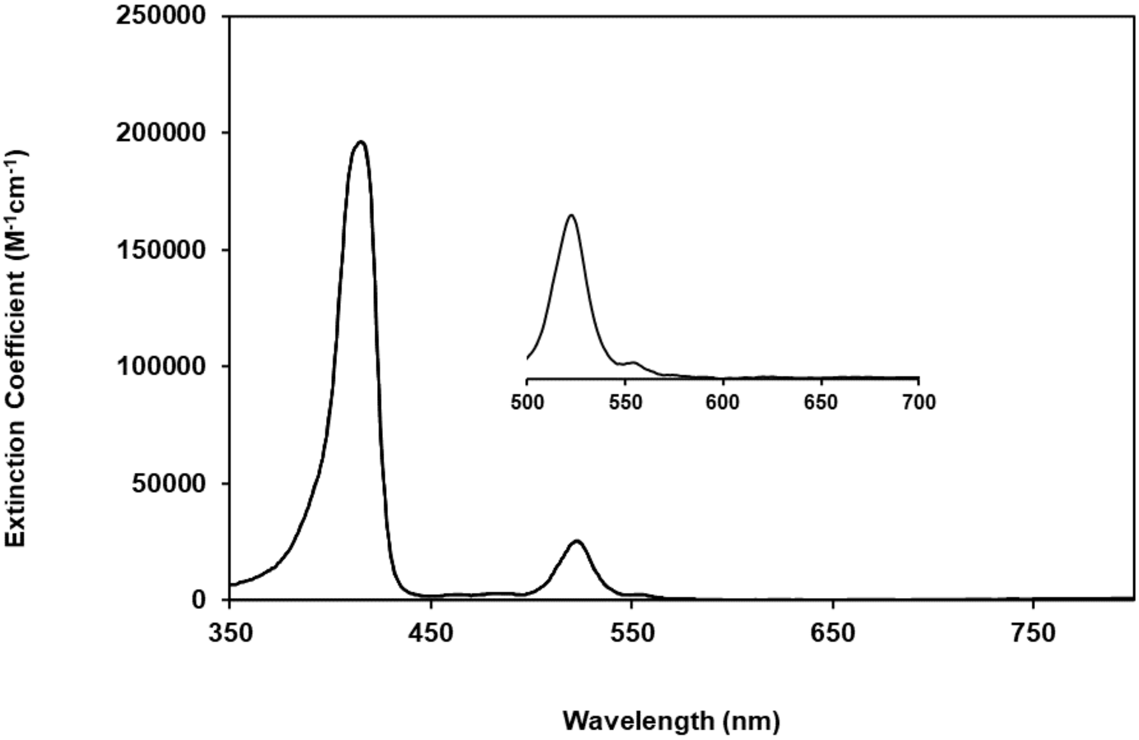


Figure S43. UV/Vis (CH_2Cl_2, rt) for **PdTPP**.

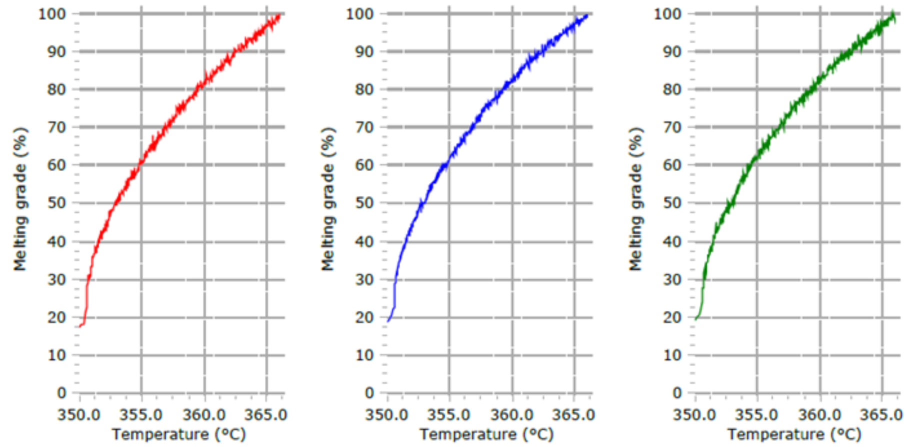
Method	(M)TPP
Start temperature:	350 °C
Temperature gradient:	1.0 °C/min
Melting result:	acc. EU pharmacopoeia
Sample ID:	PdTPP

Automatic:

Left	Center	Right
358.5 °C	363.4 °C	365.5 °C

Average: 362.5 °C

Standard deviation: 3.60 °C



Manual:

	Left	Center	Right
1:			
2:			
3:			

Figure S44. Melting point measurement of **PdTPP**.

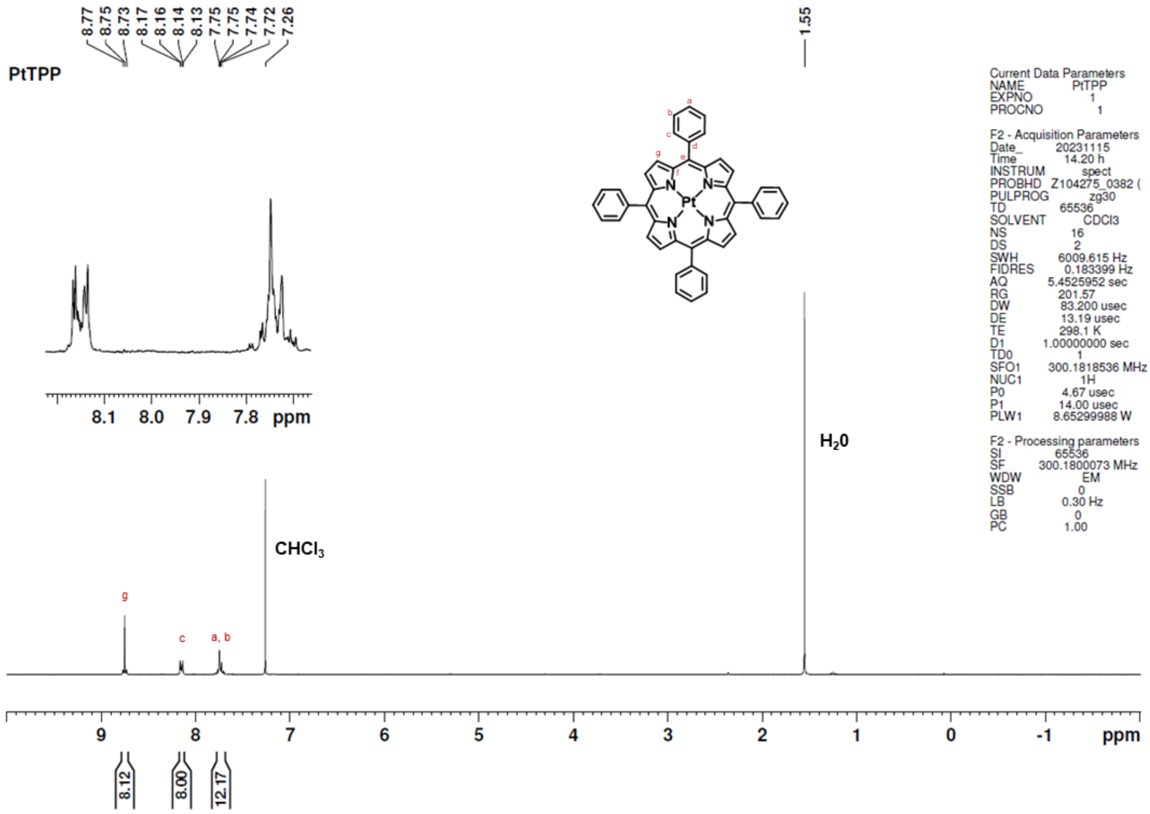


Figure S45. ^{1}H NMR (300 MHz, $CDCl_3$, rt) of **PtTPP**.

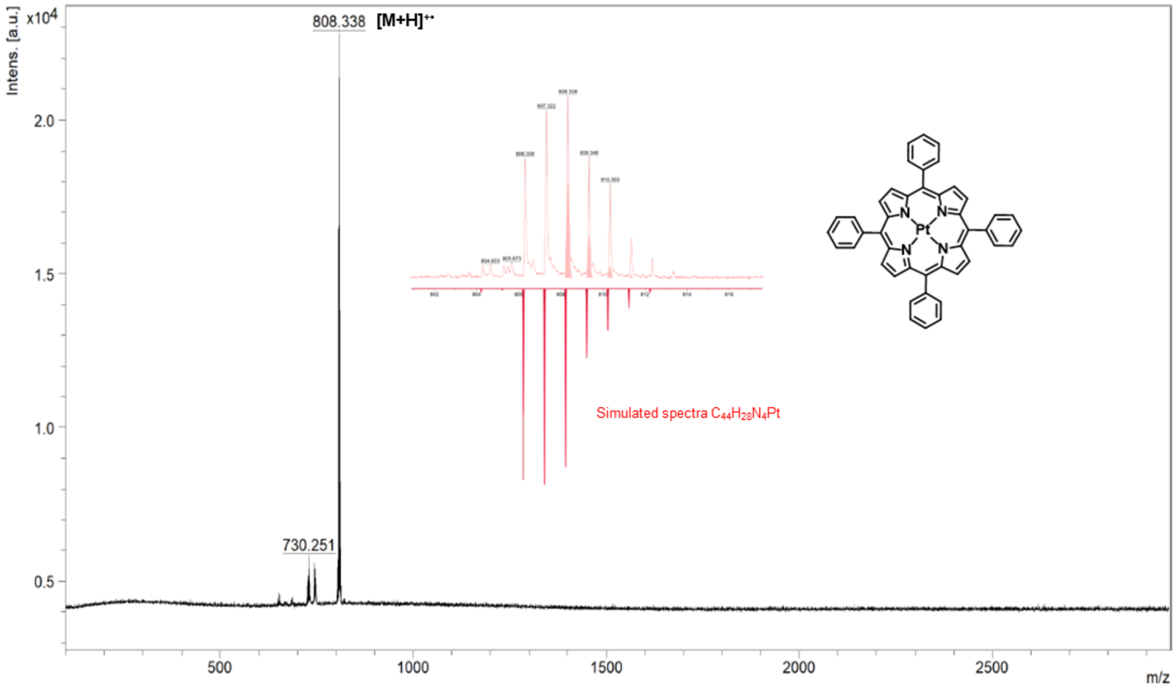


Figure S46. MS (MALDI-TOF, DCTB) of **PtTPP**.

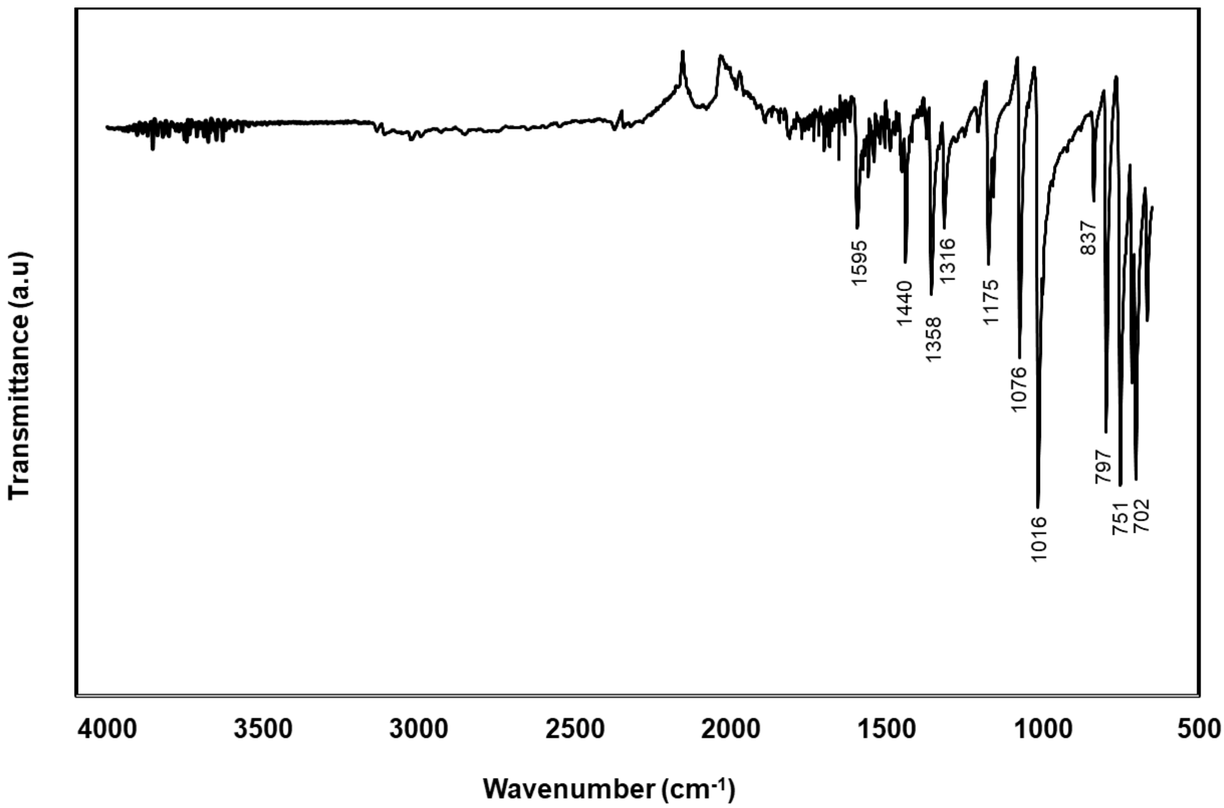


Figure S47. IR (ATR) of **PtTPP**.

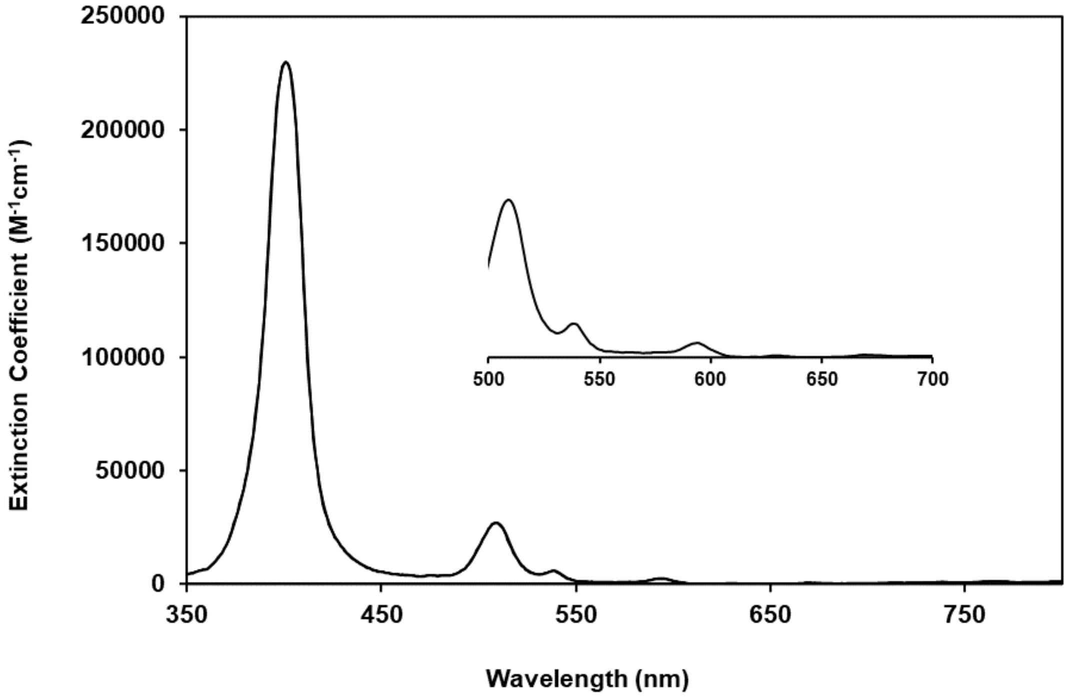


Figure S48. UV/Vis (CH_2Cl_2, rt) for **PtTPP**.

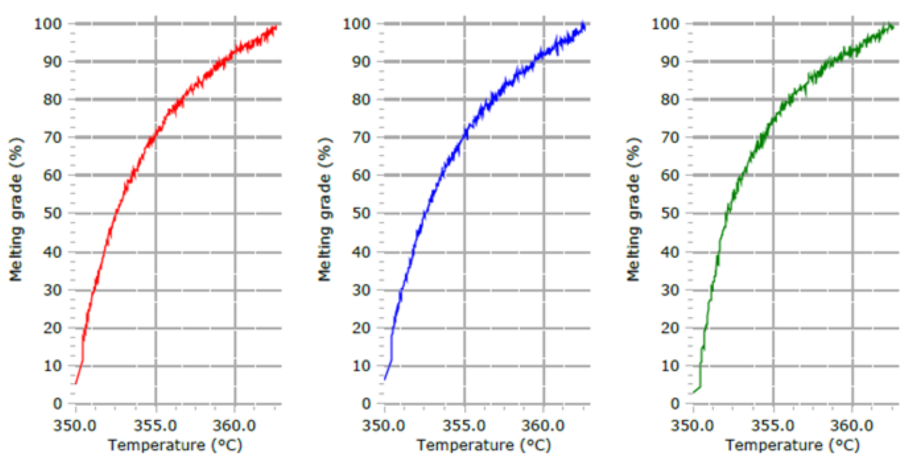
Method	(M)TPP
Start temperature:	350 °C
Temperature gradient:	1.0 °C/min
Melting result:	acc. EU pharmacopoeia
Sample ID:	PtTPP

Automatic:

Left	Center	Right
360.3 °C	361.9 °C	362.0 °C

Average: 361.4 °C

Standard deviation: 0.98 °C



Manual:

	Left	Center	Right
1:			
2:			
3:			

Figure S49. Melting point measurement of **PtTPP**.

5 Supporting References

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