Electronic Supplementary Material (ESI) for Materials Advances.

ELECTRONIC SUPPLEMENTARY INFORMATION

Metallophthalocyanines in a ternary photoactive layer (P3HT:MPc:$PC_{70}BM$) for bulk heterojunction solar cells

Denisha Gounden, Michael N. Pillay, Timo Raab, Nolwazi Nombona, Lukas Schmidt-Mende and Werner E. van Zyl

CONTENTS

(a) Elemental analysis report

INSTALLATION TEST - 25_03_2019
varioELcube
serial number: 19181072

Text report

No.	Name	N [%]	C [%]	H [%]	S [%]
22	Ligand 2	23.41	54.78	1.95	0.128

INSTALLATION TEST - 25_03_2019
varioELcube
serial number: 19181072

Text report

No.	Name	N [%]	C [%]	H [%]	S [%]
12	Ligand A	10.09	77.89	6.048	0.254
13	Ligand B	10.31	79.31	3.804	0.091
14	Ligand C	10.74	72.65	3.835	0.062
15	Ligand D	11.27	64.58	2.954	0.059

INSTALLATION TEST - 25_03_2019
varioELcube
serial number: 19181072

Text report

No.	Name	O [%]	Date Time
12	Ligand A	6.697	2020/03/13 12:08
13	Ligand B	7.046	2020/03/13 12:19
14	Ligand C	12.884	2020/03/13 12:31
15	Ligand D	21.150	2020/03/13 12:42

(b) FT-IR spectra

The FT-IR spectrum (Figure S1) of compound 1 shows a C≡N band at 2239 cm^{-1} and two intense, characteristics bands at 1535 cm^{-1} and 1345 cm^{-1} corresponding to the asymmetric and symmetric stretching of the NO_2 functional group respectively. The conversion of compound 1 to compounds **2a, 2b, 2c** and **2d** were confirmed by the disappearance of the NO_2 bands and the appearance of bands in the 1244 - 1248 cm^{-1} region belonging to the newly formed diaryl ether linkage (C-O-C) (Figure S1). The FT-IR spectra for all 16 metal phthalocyanines can be viewed in the supplementary materials section (Figures S2-S5) and show an expected disappearance of the C≡N band indicating the conversion of the dinitrile precursors to metal Pcs. Bands appearing in the 1240 – 1220 cm^{-1} region confirm the peripherally attached substituents. Table S1 provides detailed band assignment for the C-H, C-C and C-N originating from the phthalocyanine skeleton.

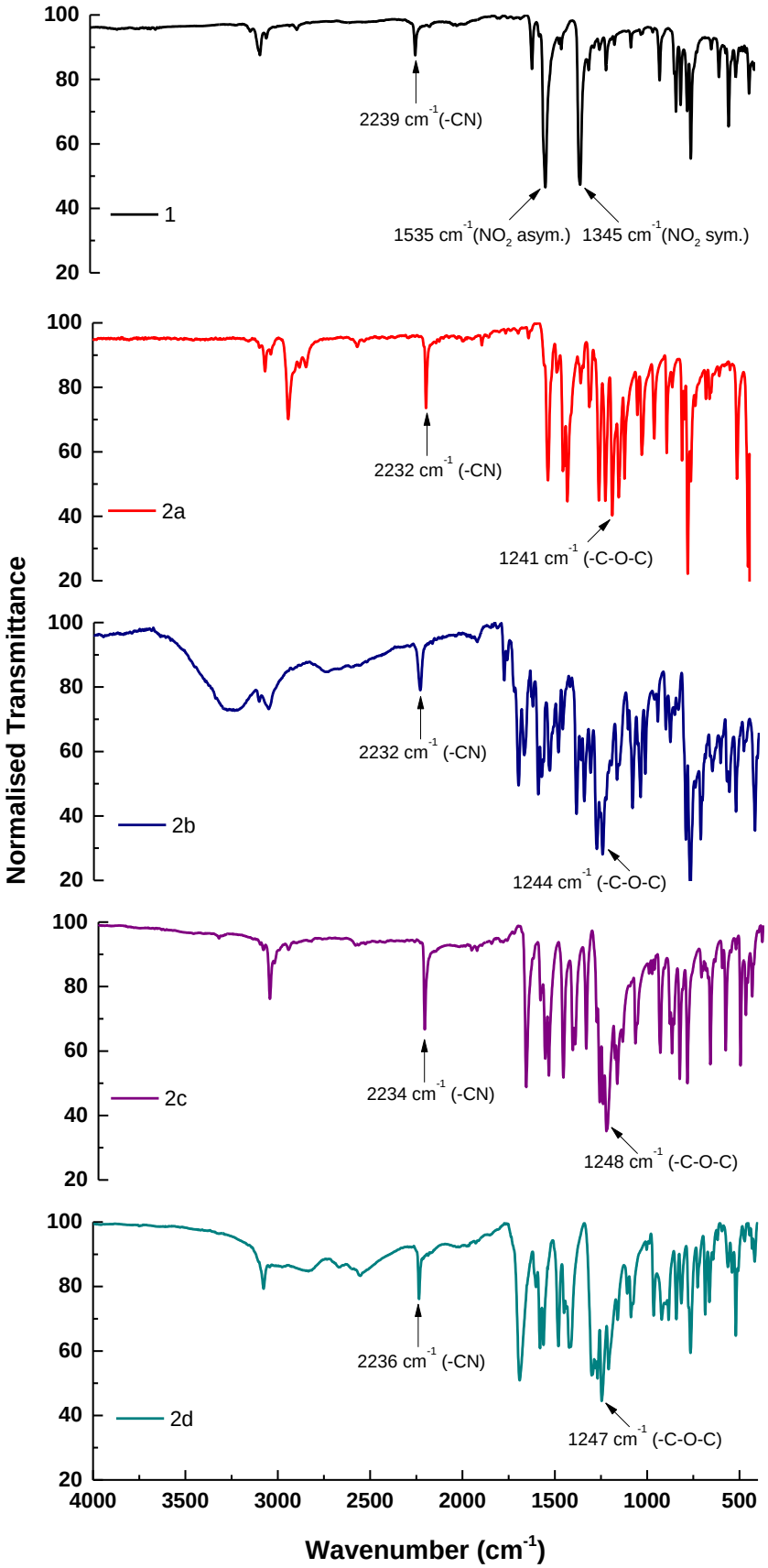


Figure S1. FT-IR spectra of 4-nitrophthalonitrile **(1)** and substituted phthalonitriles **(2a-2d)**.

Table S1. FTIR absorption bands (cm-1) of MPc complexes (3a-3d, 4a-4d, 5a-5d and 6a-6d).

Band Assignment (cm^{-1})												
Metal complex	**C-H sym.**	**C-H asym.**	**C-C stretch (pyrrole)**	**C-H (aryl)**	**C-C (isoindole)**	**C-O-C**	**C-N (β^{**})**	**C-H bend (β^{**})**	**C-N stretch (pyrrole)**	**C-H deform. (γ^{**})**	**C-H deform. (γ^{**})**	**C-N stretch**
3a	2958	2865	1602	1467	1334	1237	1175	1081	1052	890	870	745
3b	2959	2850	1605	1466	1333	1233	1161	1093	1063	908	874	750
3c	2958	2865	1599	1471	1329	1237	1169	1070	1050	890	870	746
3d	2958	2866	1597	1465	1332	1231	1163	1073	1049	895	871	745
4a	2920	2850	1604	1461	1337	1237	1164	1094	1056	908	878	747
4b	2922	2857	1595	1457	1324	1224	1151	1088	1056	913	879	744
4c	2927	2853	1596	1455	1324	1221	1152	1070	1048	909	872	743
4d	2926	2851	1595	1459	1331	1227	1150	1072	1050	903	871	743
5a	2919	2851	1604	1463	1336	1237	1166	1093	1057	907	878	750
5b	2921	2855	1594	1458	1325	1221	1155	1086	1055	909	878	745
5c	2925	2855	1594	1457	1326	1220	1153	1068	1050	911	874	744
5d	2927	2853	1594	1461	1328	1225	1151	1072	1049	902	872	745
6a	2927	2865	1600	1459	1331	1229	1163	1092	1052	895	875	747
6b	2921	2853	1604	1467	1332	1232	1160	1093	1059	908	880	750
6c	2921	2853	1603	1467	1331	1228	1159	1094	1066	908	871	750
6d	2929	2856	1597	1464	1332	1230	1163	1072	1050	895	873	745

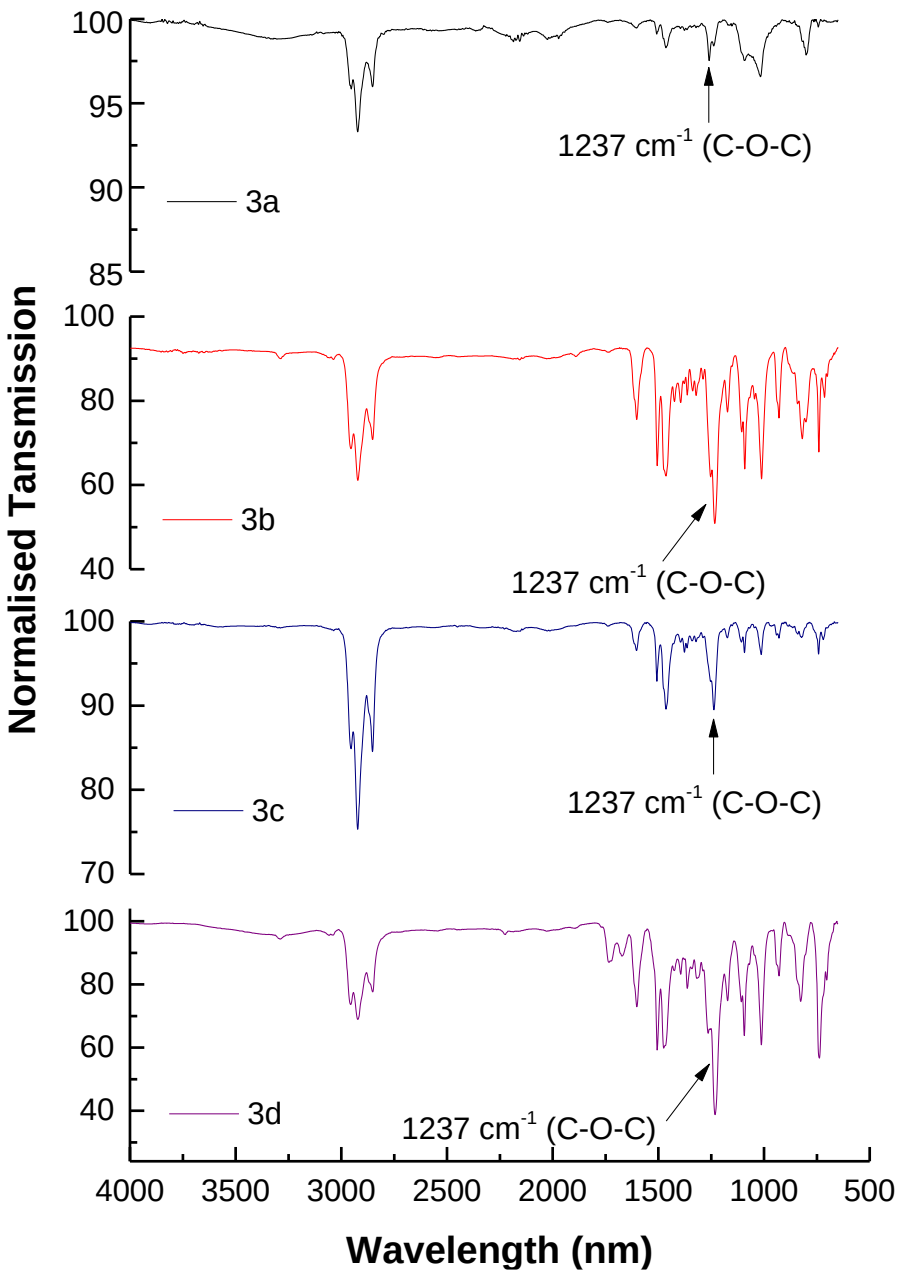


Figure S2. FT-IR spectra of CoPc complexes **(3a-3d)**.

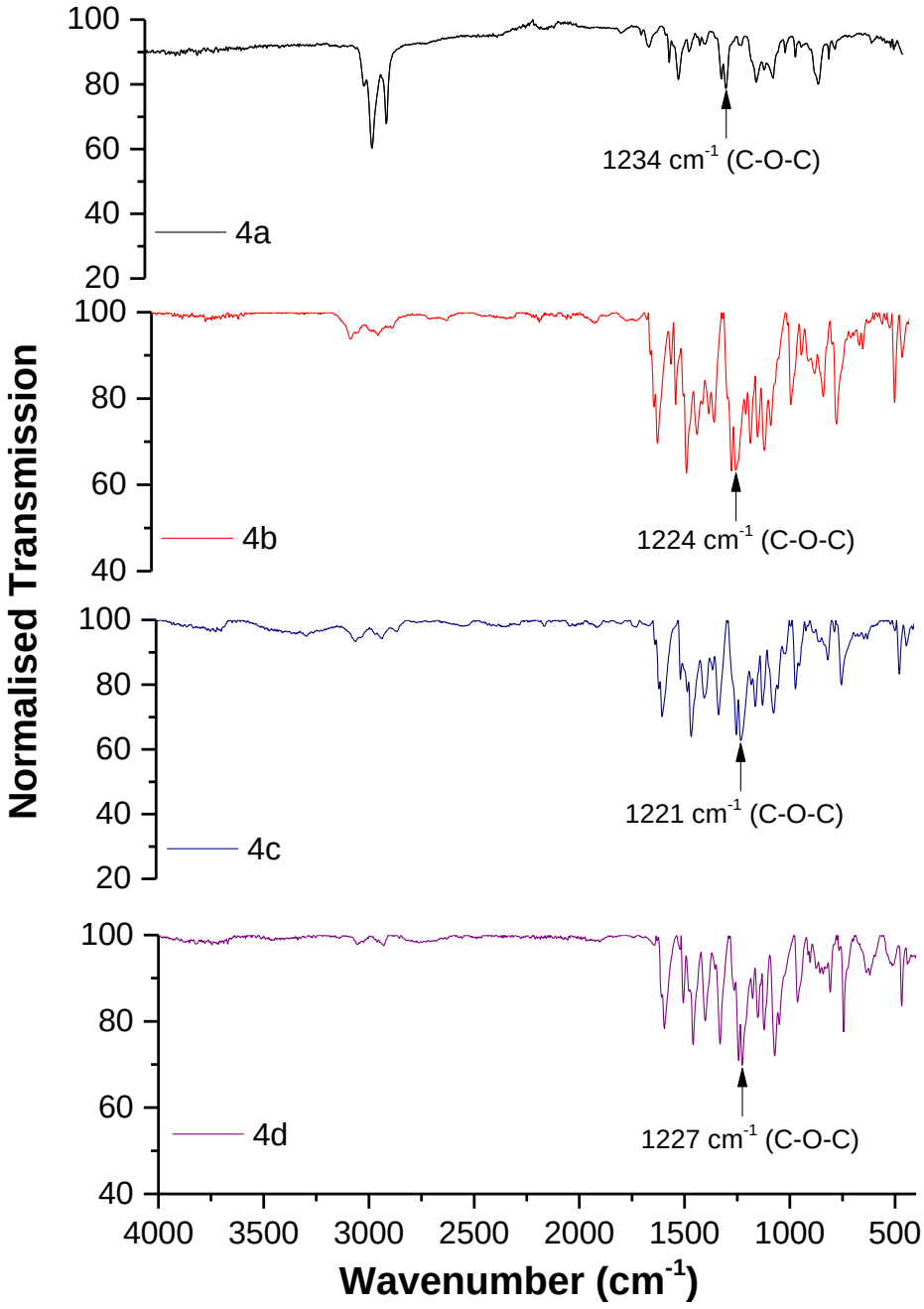


Figure S3. FT-IR spectra of NiPc complexes **(4a-4d)**.

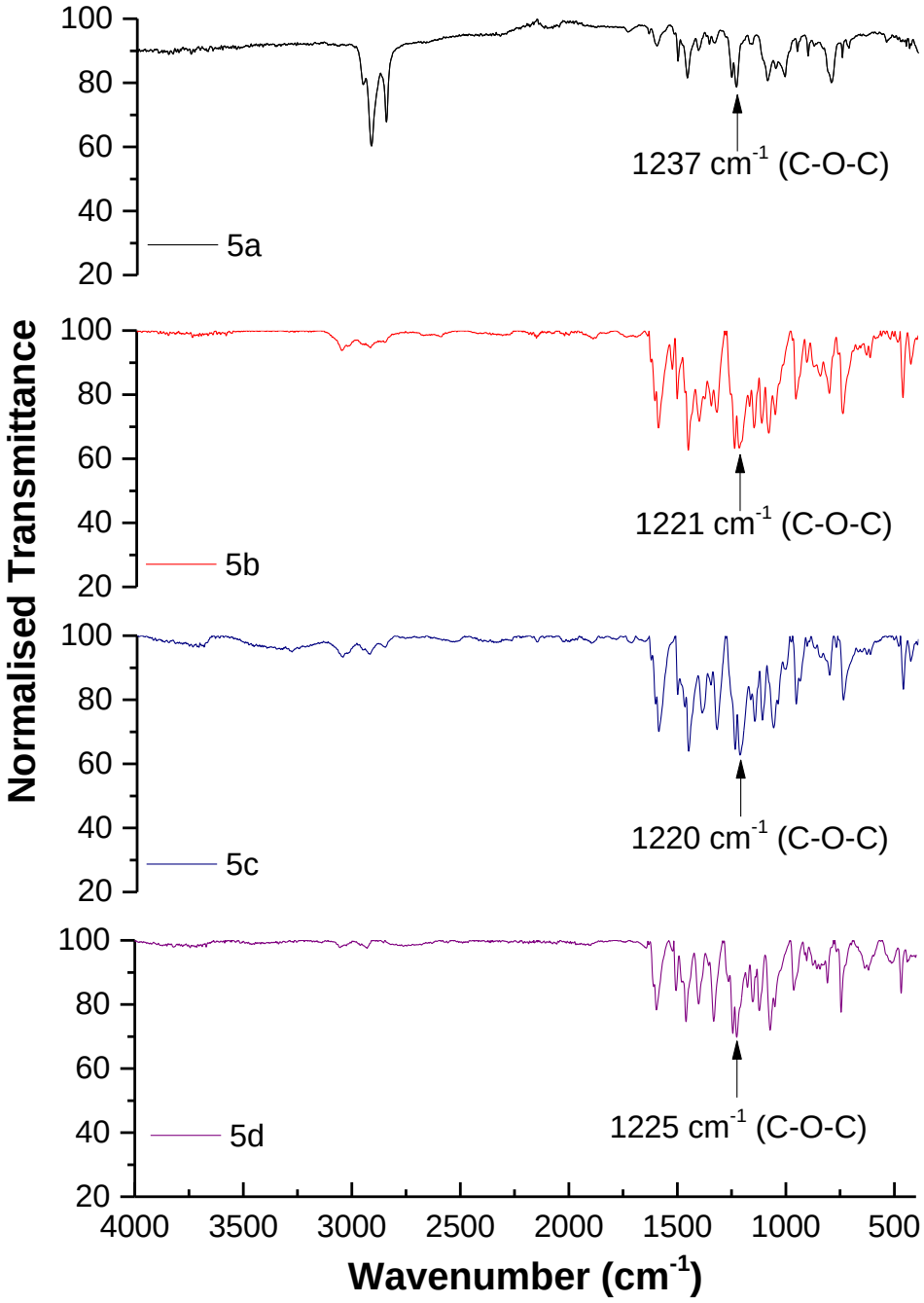


Figure S4. FT-IR spectra of TiPc complexes **(5a-5d)**.

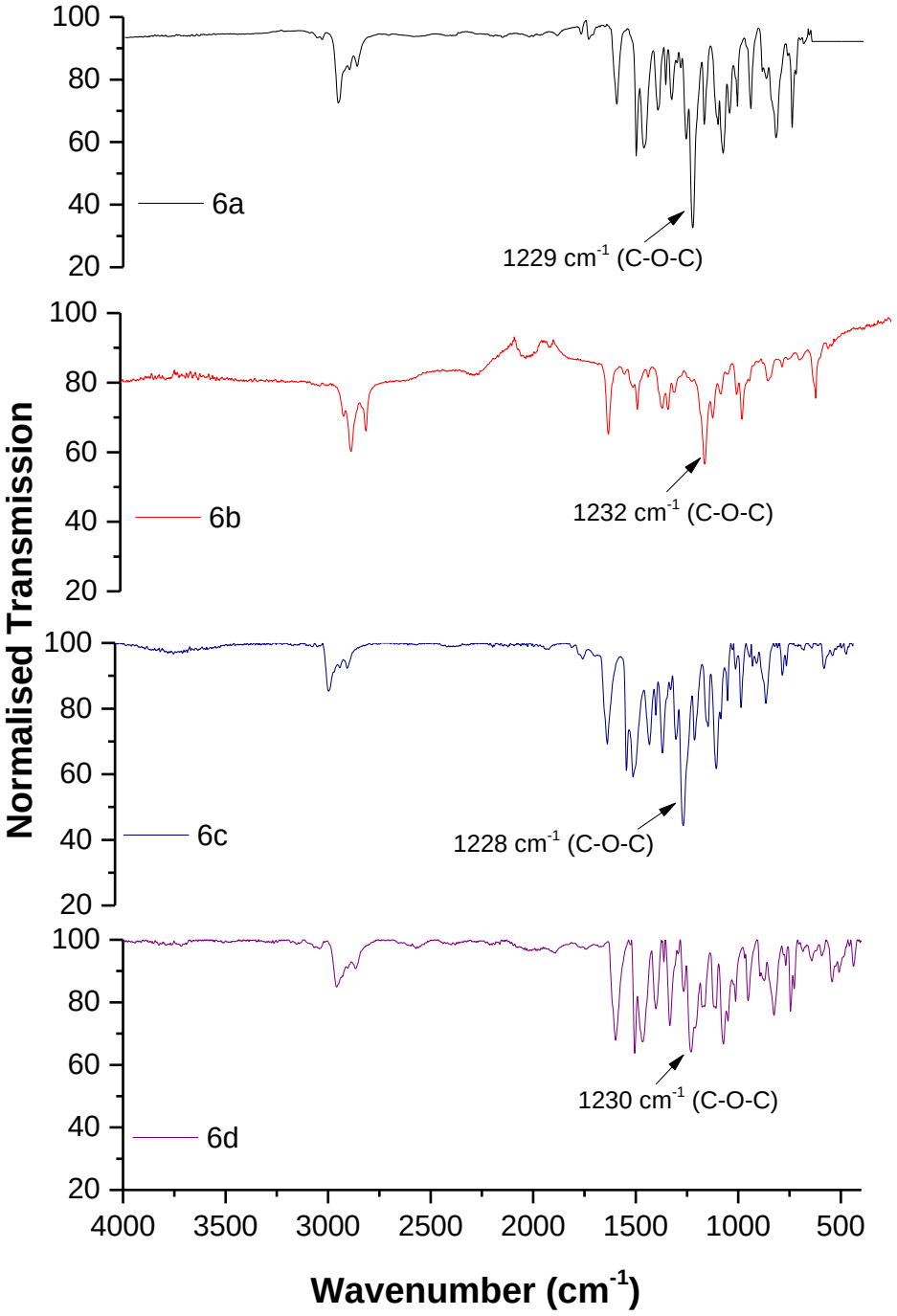


Figure S5. FT-IR spectra of MnPc complexes **(6a-6d)**.

(c) Mass spectroscopy

The MALDI-TOF spectra (Figures S6-S9) provided evidence for the successful synthesis of complexes **3a-3d, 4a-4d** and **5a-5d** with molecular ion peaks that match well with the calculated molecular weights. Molecular ion peaks for Mn containing complexes (**6a-6d)**, were not observed in the MALDI-TOF spectra. However, base peaks corresponding to MnPcs with cleaved axial Mn-Cl bonds were detected at 1162, 1138, 1105, 1114 *m/z* respectively.

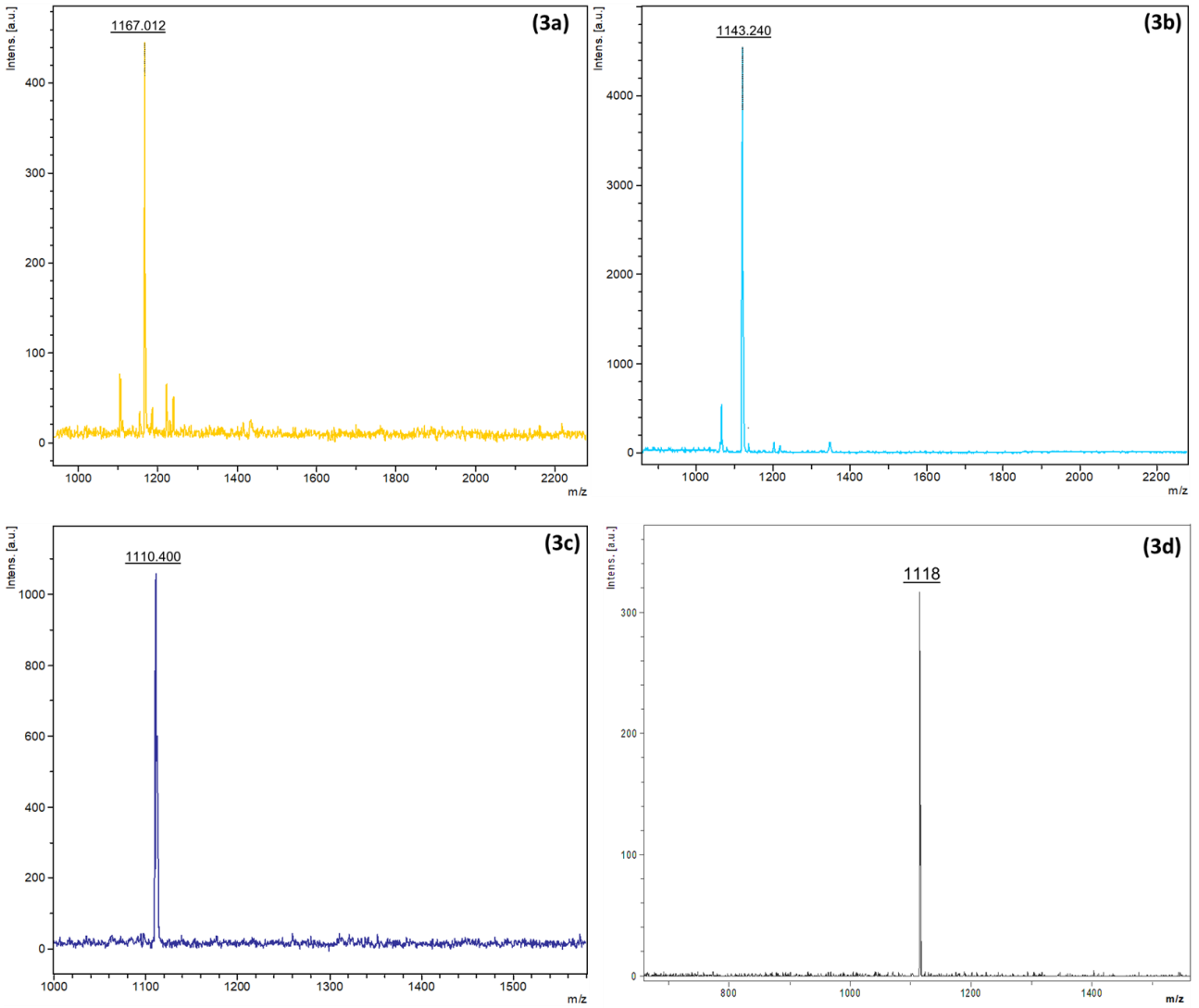


Figure S6. Mass spectra of CoPc complexes **(3a-3d)**.

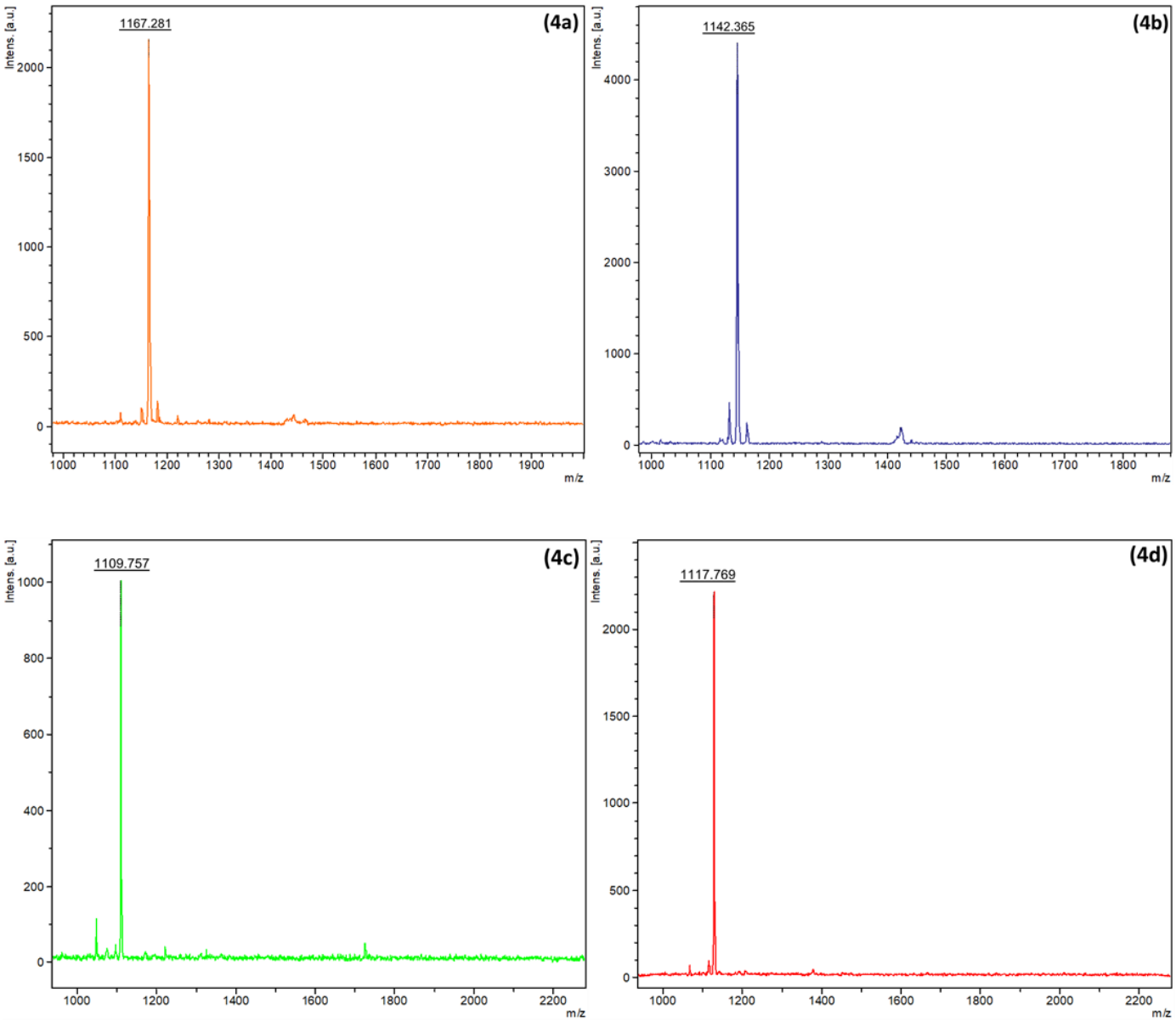


Figure S7. Mass spectra of NiPc complexes **(4a-4d)**.

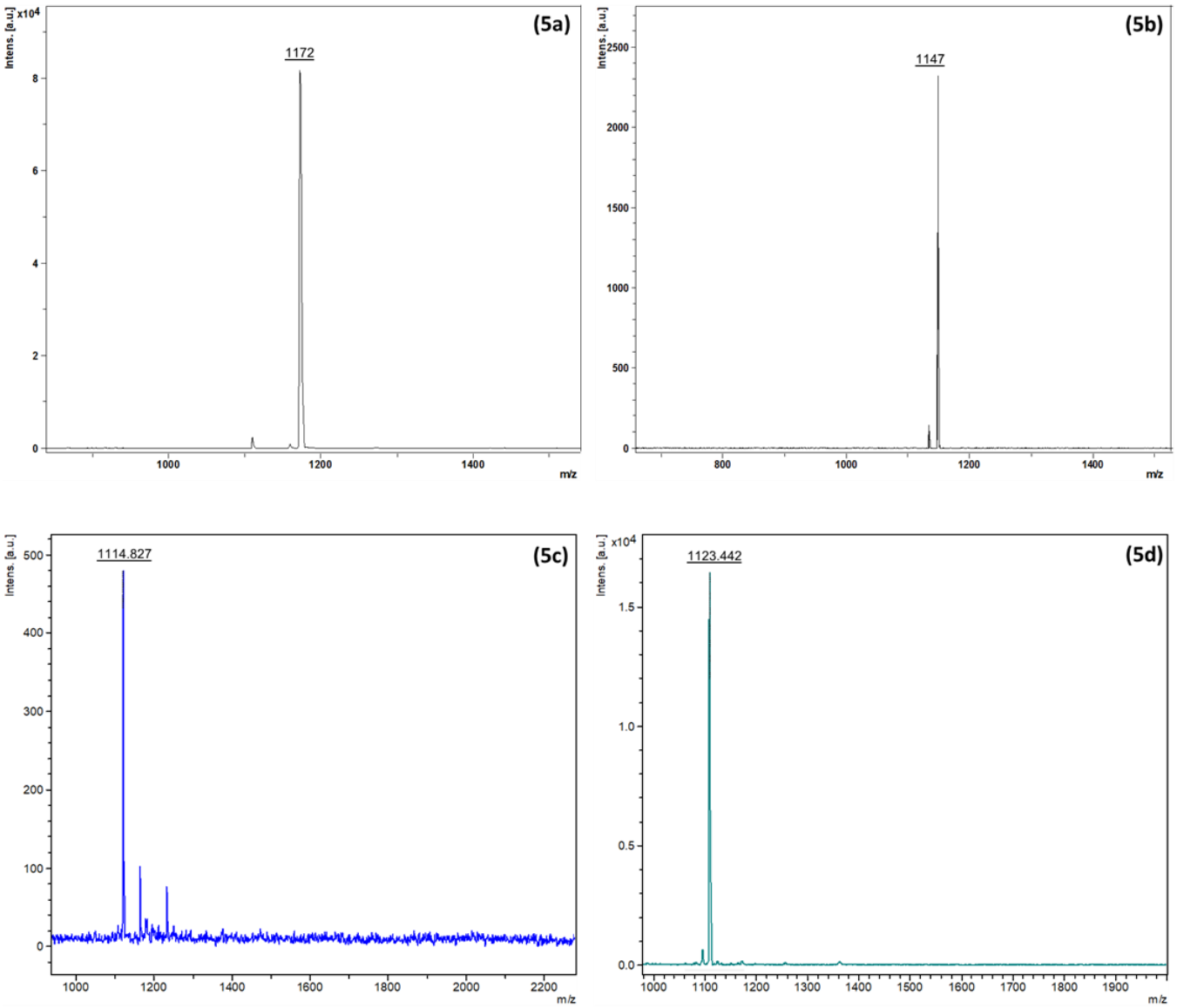


Figure S8. Mass spectra of TiPc complexes **(5a-5d)**.

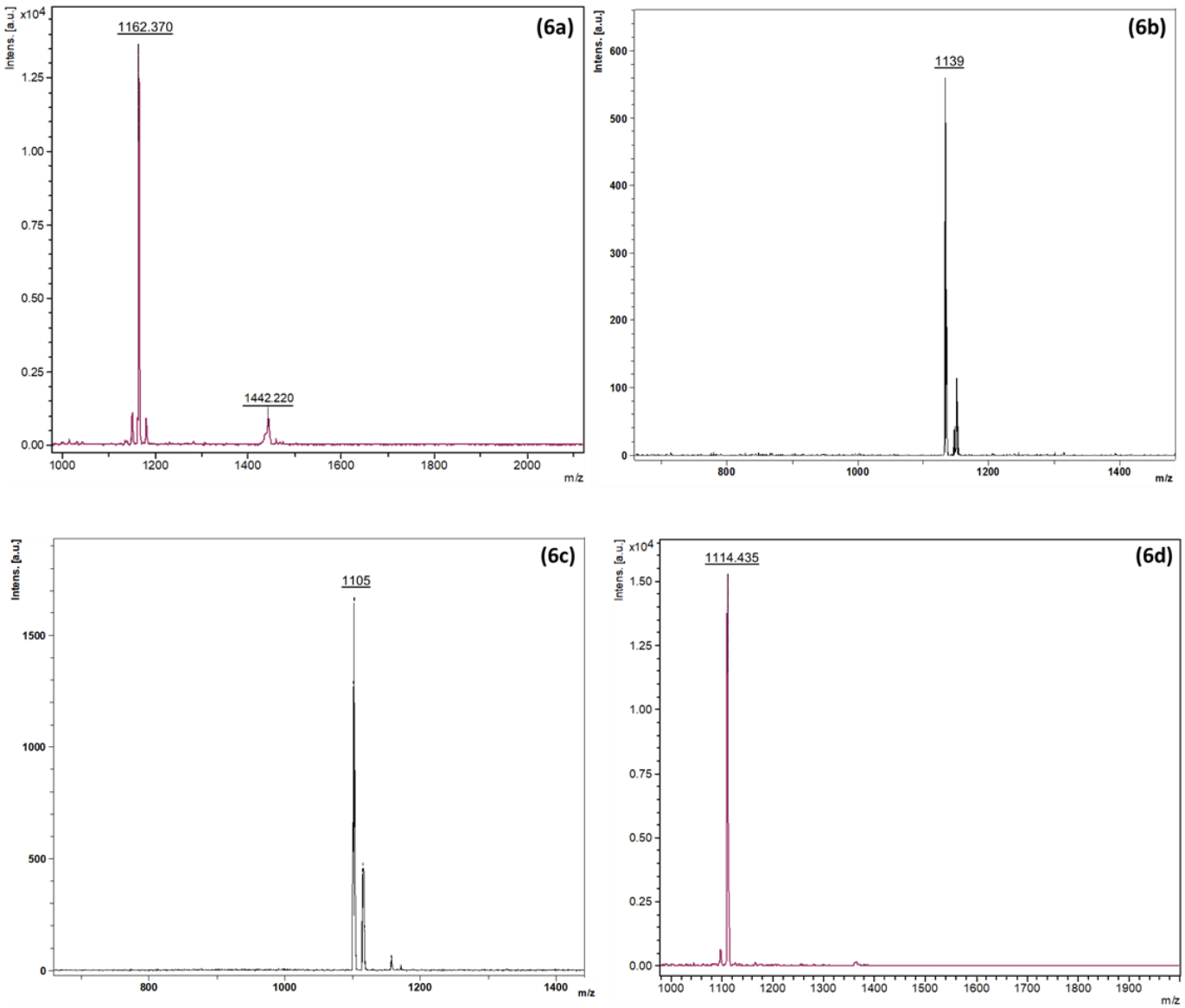


Figure S9. Mass spectra of MnPc complexes **(6a-6d)**.

(d) UV-vis spectroscopy

Table S2. Main UV-vis absorption maxima of the Co, Ni, Ti and Mn Pcs in solution (solvent: CH_3Cl[a] or THF[b]) and solid-state.

Metal	Substituent	Solution				Solid	
		Q (nm)	VB (nm)	B (nm)	CT band	Q (nm)	B (nm)
Co	**1**[a]	672	607	325	×	614	360
	2[a]	672	607	326	×	619	361
	3[a]	669	605	320	×	614	370
	4[a]	672	605	322	×	619	×
Ni	**1**[b]	674	607	329	✓	608	369
	2[b]	674	607; 646	328	✓	614	367
	3[b]	673	607; 644	329	✓	617	363
	4[b]	673	608; 644	328	✓	611	358
Ti	**1**[a]	704	634	346	✓	700	360
	2[a]	703	668; 634	346	✓	707	360
	3[a]	702	667; 636	341	✓	700	360
	4[a]	701	666; 634	344	✓	702	360
Mn	**1**[a]	734	662	373	✓	721	379
	2[a]	734	662	391	✓	723	367
	3[a]	719	×	353	✓	727	367
	4[a]	729	657	358	✓	718	370

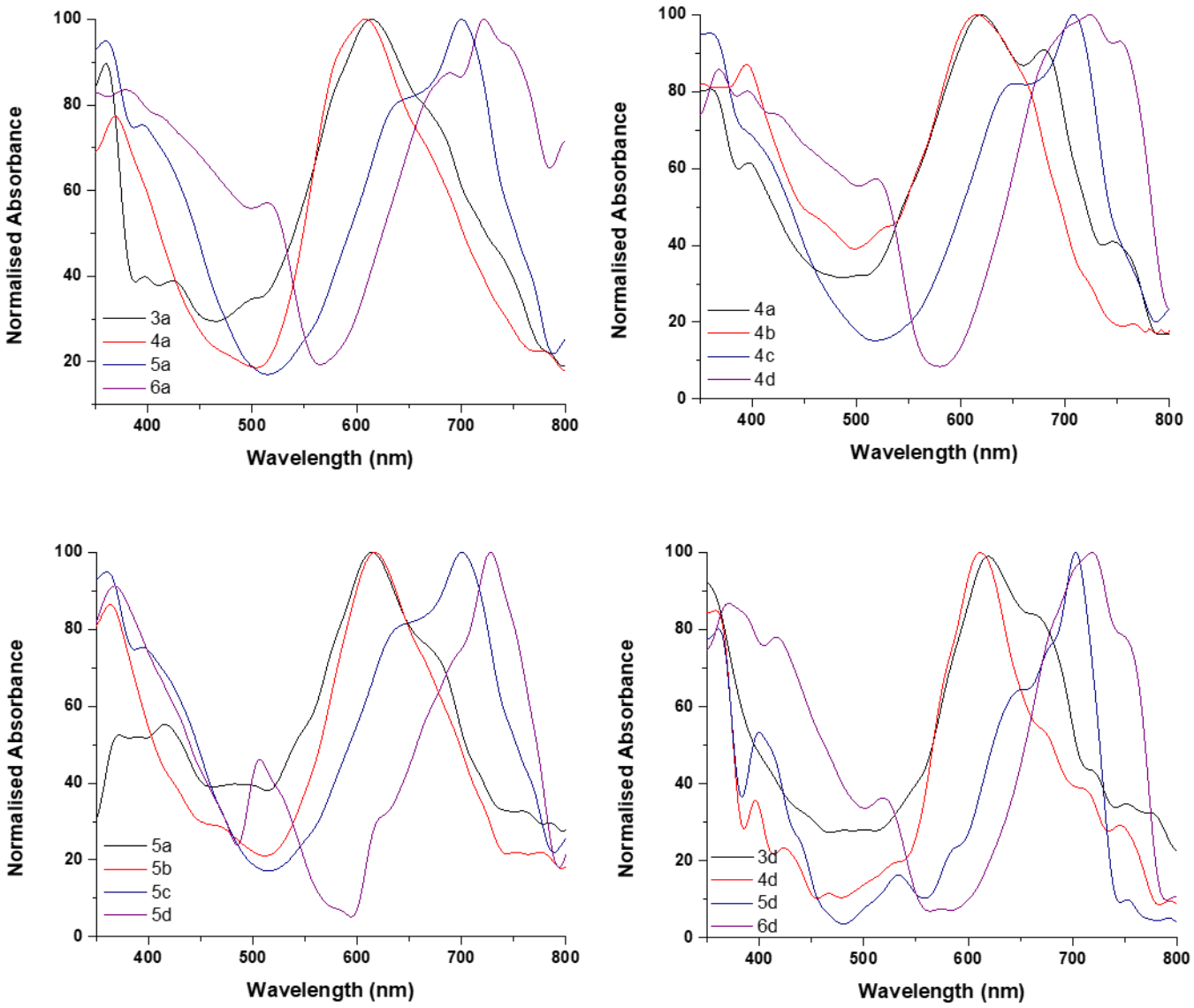


Figure S10. UV–vis absorption spectra of MPc complexes **(3a-3d, 4a-4d, 5a-5d** and **6a-6d)** spin-coated on glass substrates.

Table S3. Absorption co-efficient (ε) for CoPcs (**3a, 3c** and **3d**), TiPcs (**5a, 5c** and **5d**) and MnPcs (**6a, 6c** and **6d**).

Metal	Substituent	Absorption co-efficient (ε), M^{-1} cm^{-1}
Co	**3a**	3.54
	3c	3.47
	3d	3.46
Ti	**5a**	3.64
	5c	3.66
	5d	3.68
Mn	**6a**	3.69
	6c	3.75
	6d	3.75

(e) Bandgap energy - Tauc plots

The Tauc and Davis-Mott relationship was used to determine the optical band gap (E_g) of the MPcs and is represented by the equation below:

$$(ahv)^n = K\,(hv - E_g)$$

where α is the absorption coefficient, h is Planck's constant, v is the photon's frequency, K is an energy-dependent constant, E_g is the bandgap, and the exponent n represents the nature of the transition and may take on values $n = \frac{1}{2}, 1, \frac{3}{2}$ or 2, depending upon the nature of the electronic transitions (i.e. allowed or forbidden) responsible for the absorption. As the nature of the electronic transition between the a_{1u} and e_g energy levels is direct and allowed, a value of n = $\frac{1}{2}$ was used for the calculations. The E_g values were obtained by extrapolation of $(ahv)^{n=\frac{1}{2}} = 0$. The Tauc plots for the MPcs can viewed in Figures S11-S14 and the Tauc plots of the $PC_{70}BM$ and P3HT in Figure S15.

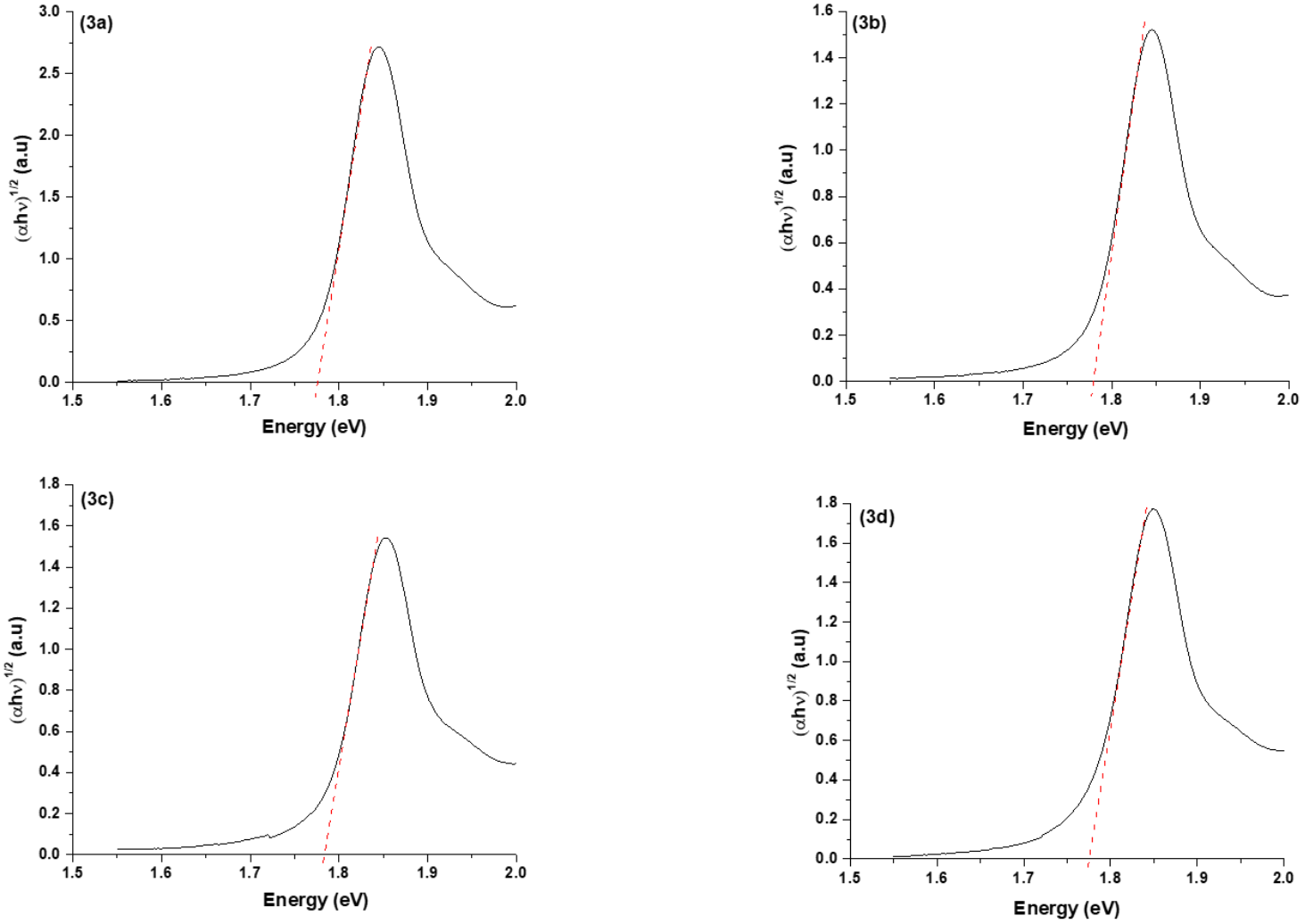


Figure S11. Tauc plots of CoPc complexes **(3a-3d)**.

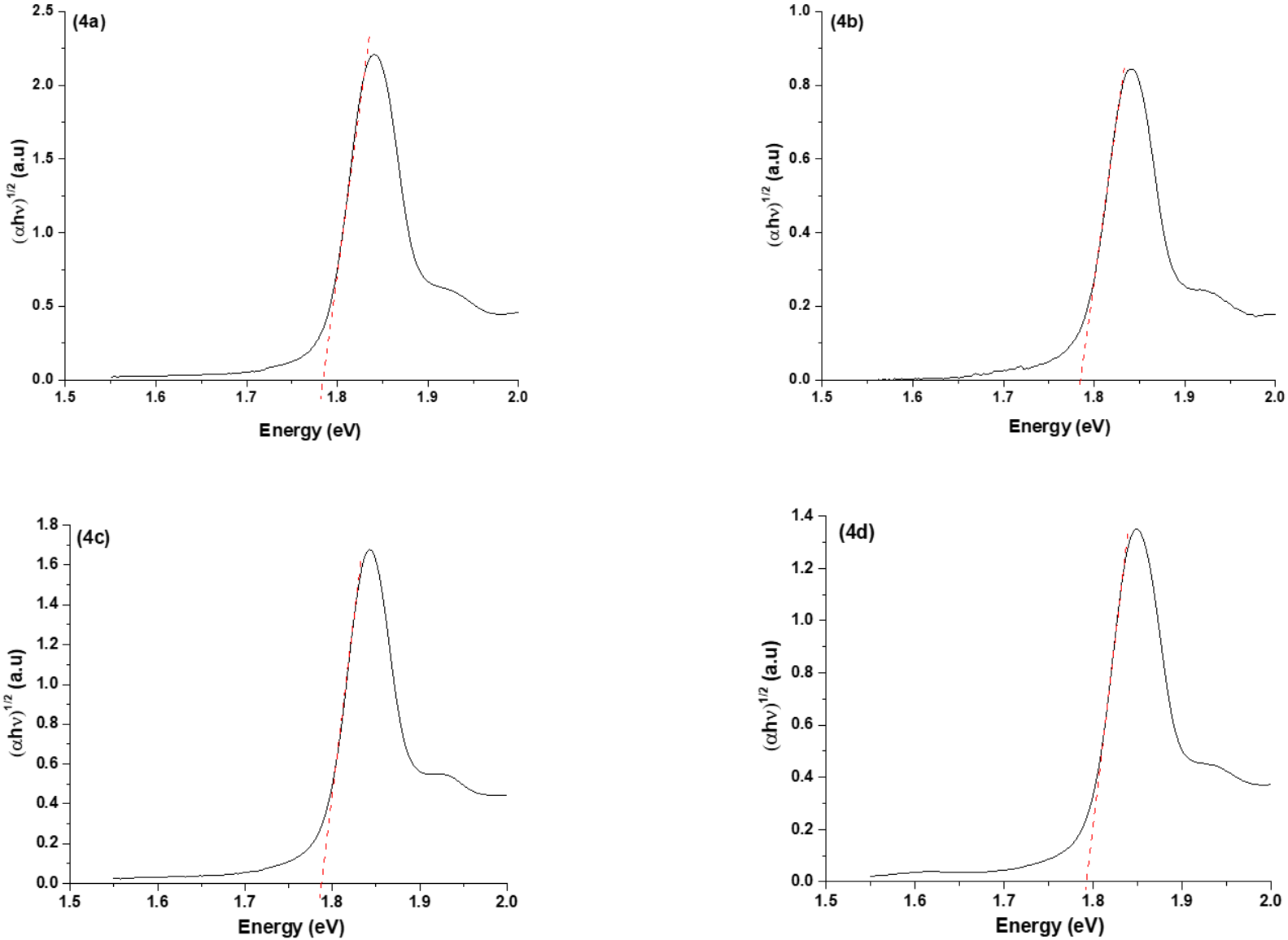


Figure S12. Tauc plots of NiPc complexes **(4a-4d)**.

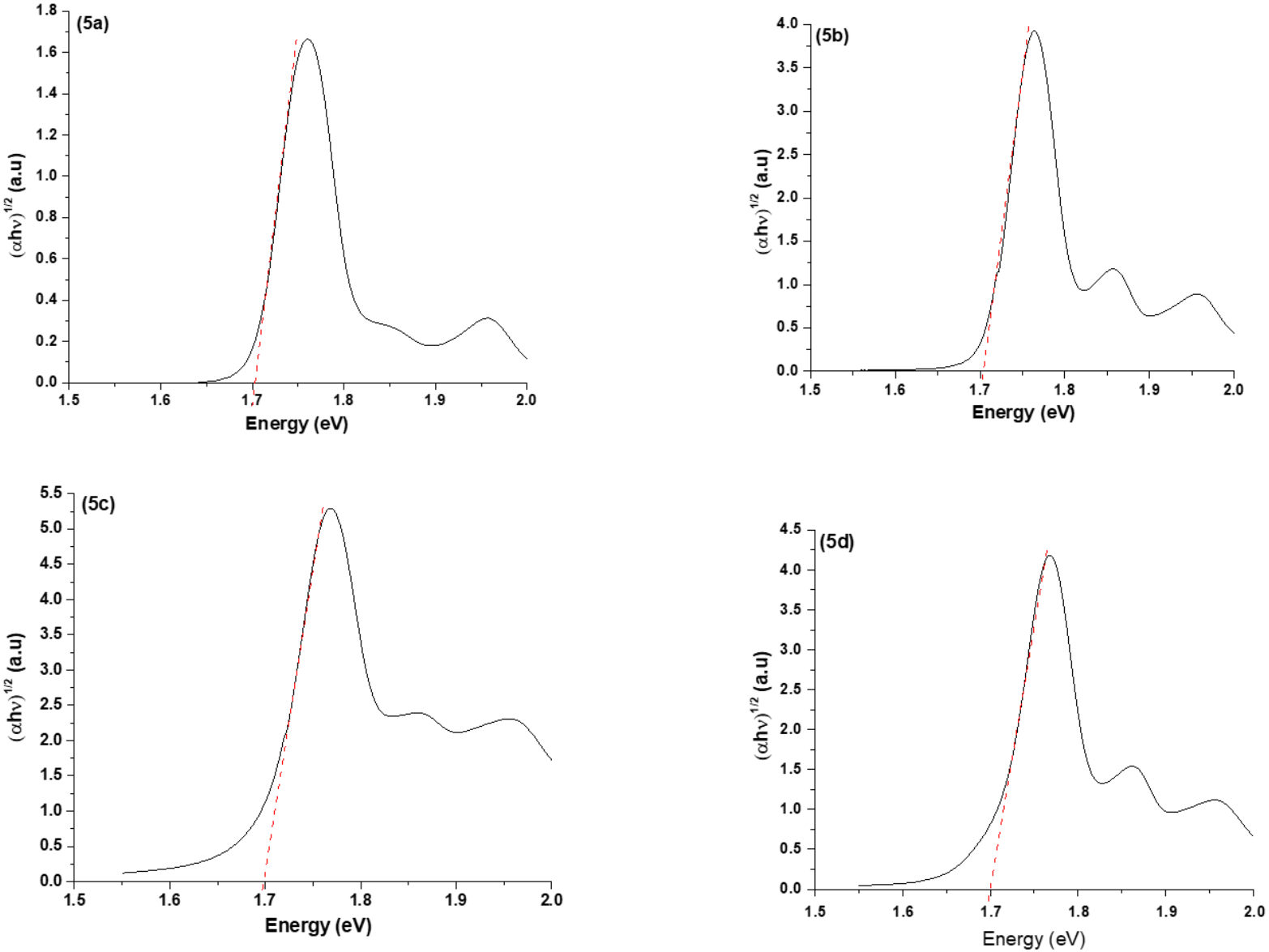


Figure S13. Tauc plots of TiPc complexes **(5a-5d)**.

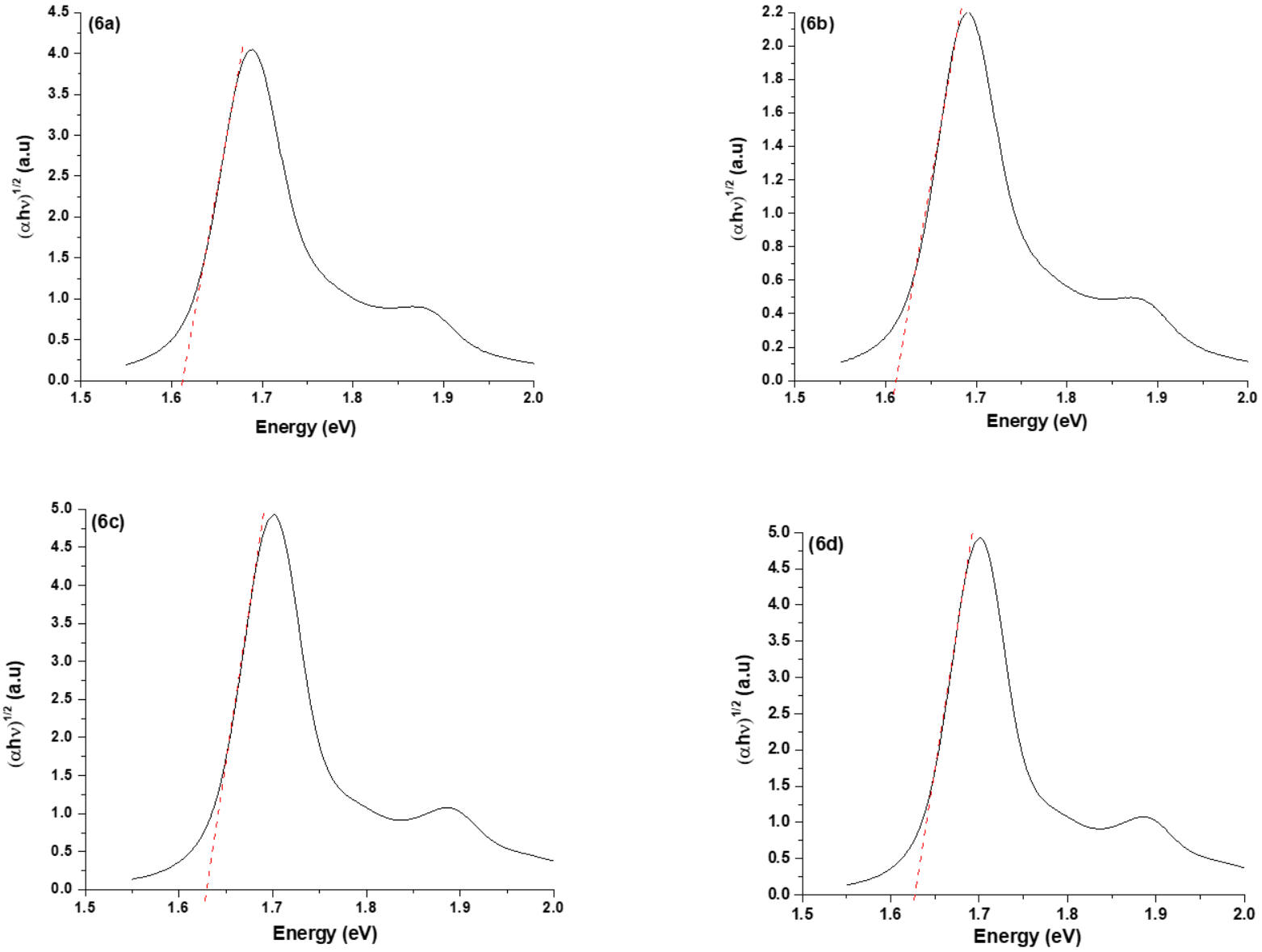


Figure S14. Tauc plots of MnPc complexes **(6a-6d)**.

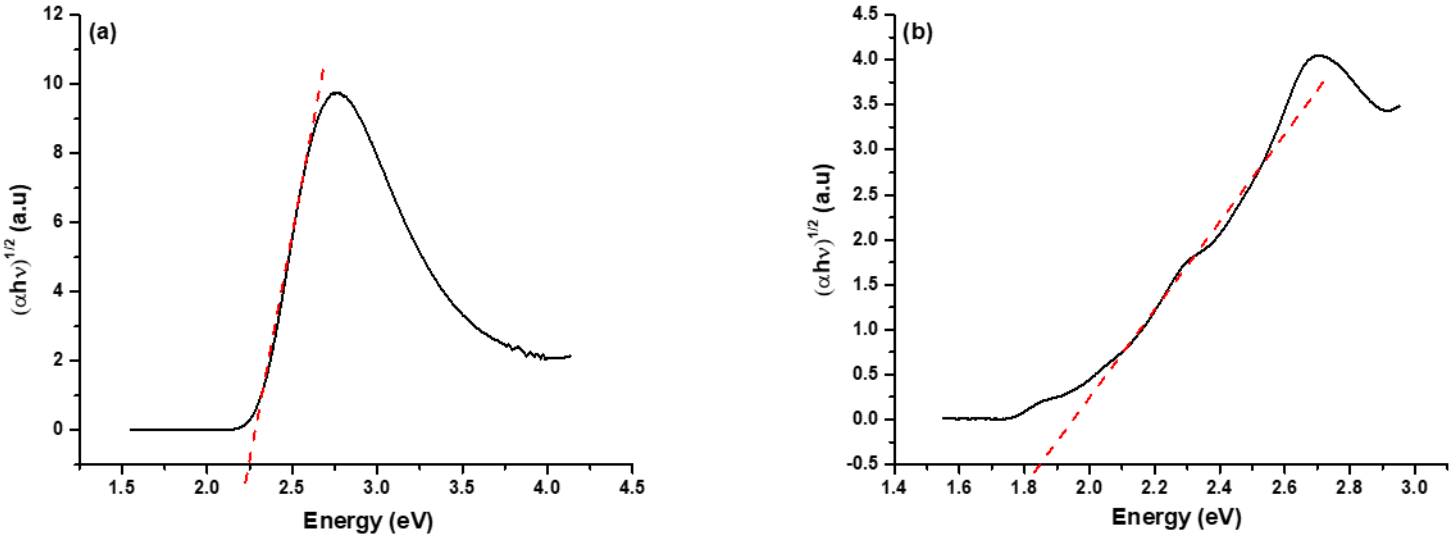


Figure S15. Tauc plots of (a) P3HT and (b) $PC_{70}BM$.

(f) HOMO energy level - Photoelectron spectroscopy in air (PESA)

PESA was used to determine the energy band structure of the MPcs. The light intensity for the PESA measurements was optimised at 15 nW for the complexes to prevent saturation of the electron counter. The IPs or HOMO levels of the complexes were measured under ambient conditions and estimated by plotting the electron count rate (n_e) against the photon energy (eV) and extrapolating to n_e = 0. These plots are shown in Figures S16-S19 for the MPcs and in Figure S20 for $PC_{70}BM$ and P3HT.

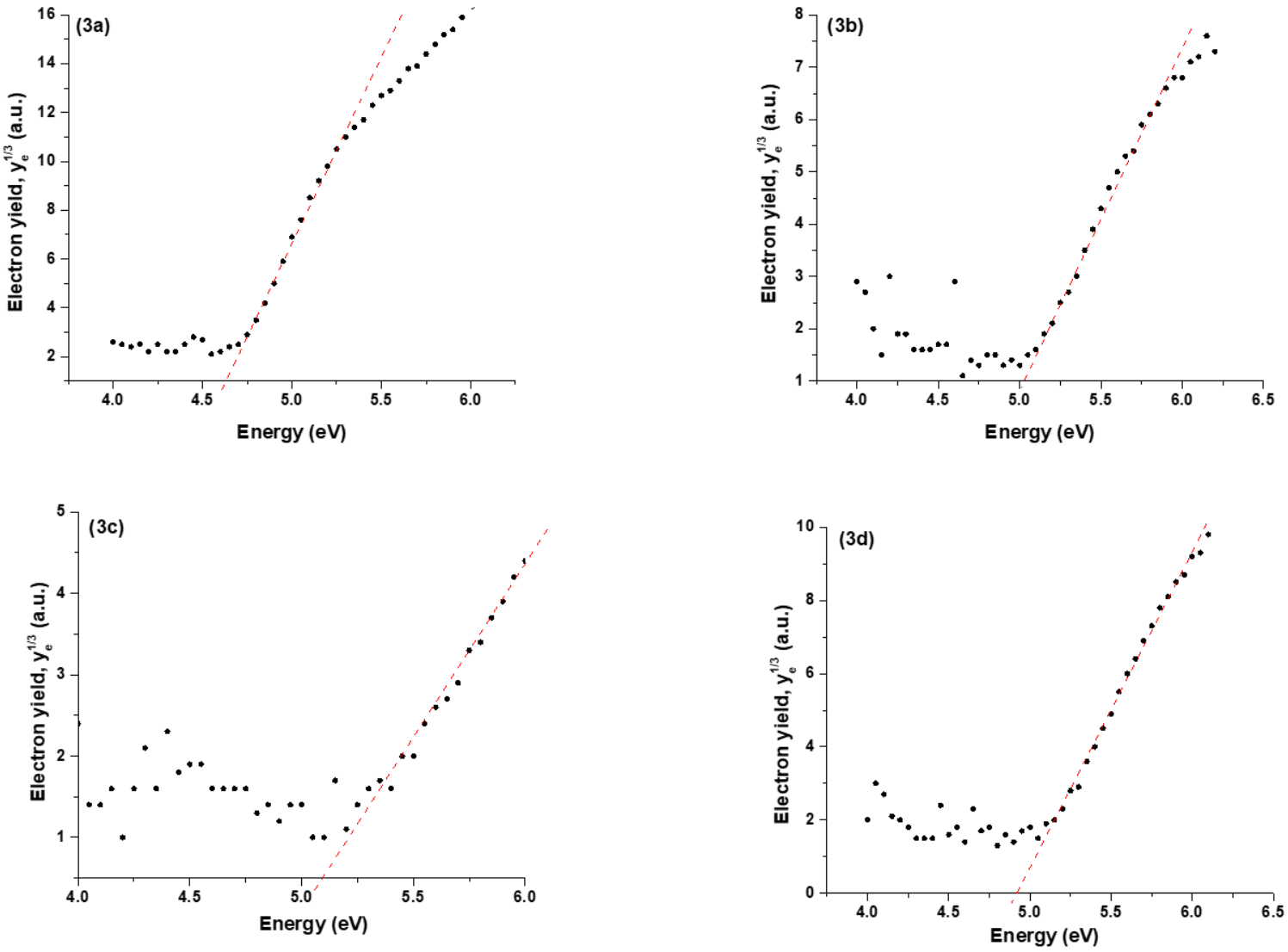


Figure S16. PESA plots of CoPc complexes **(3a-3d)**.

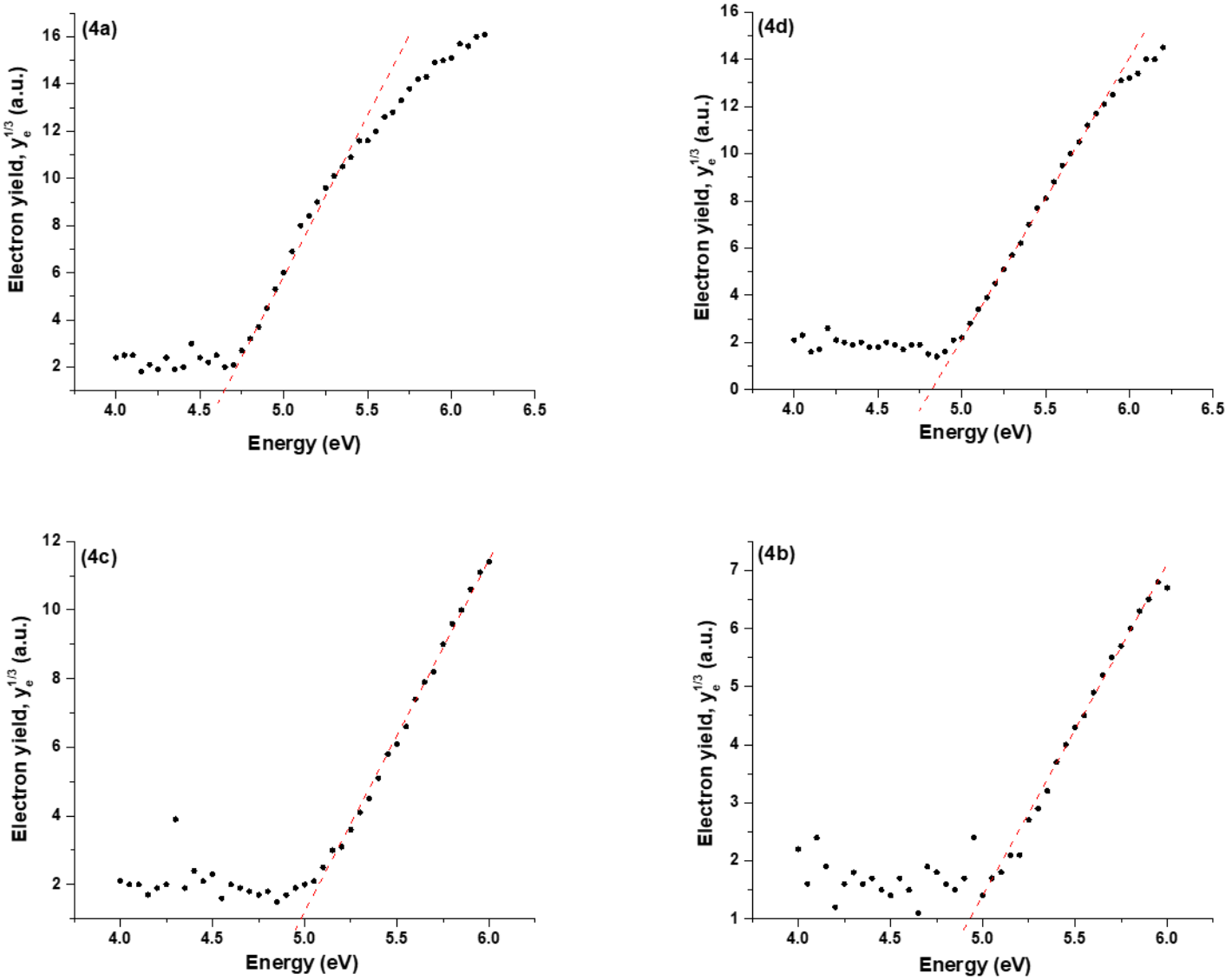


Figure S17. PESA plots of NiPc complexes **(4a-4d)**.

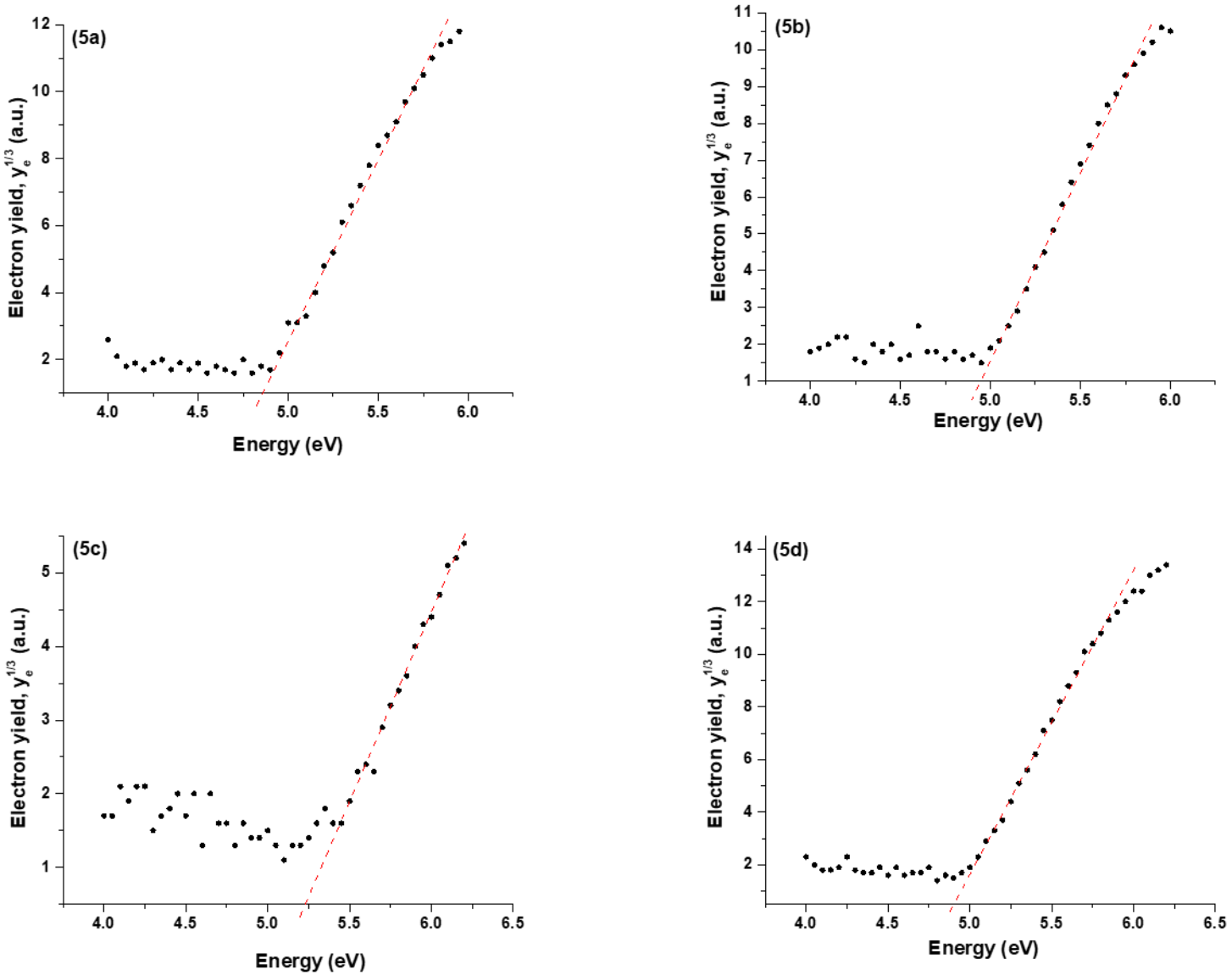


Figure S18. PESA plots of TiPc complexes **(5a-5d)**.

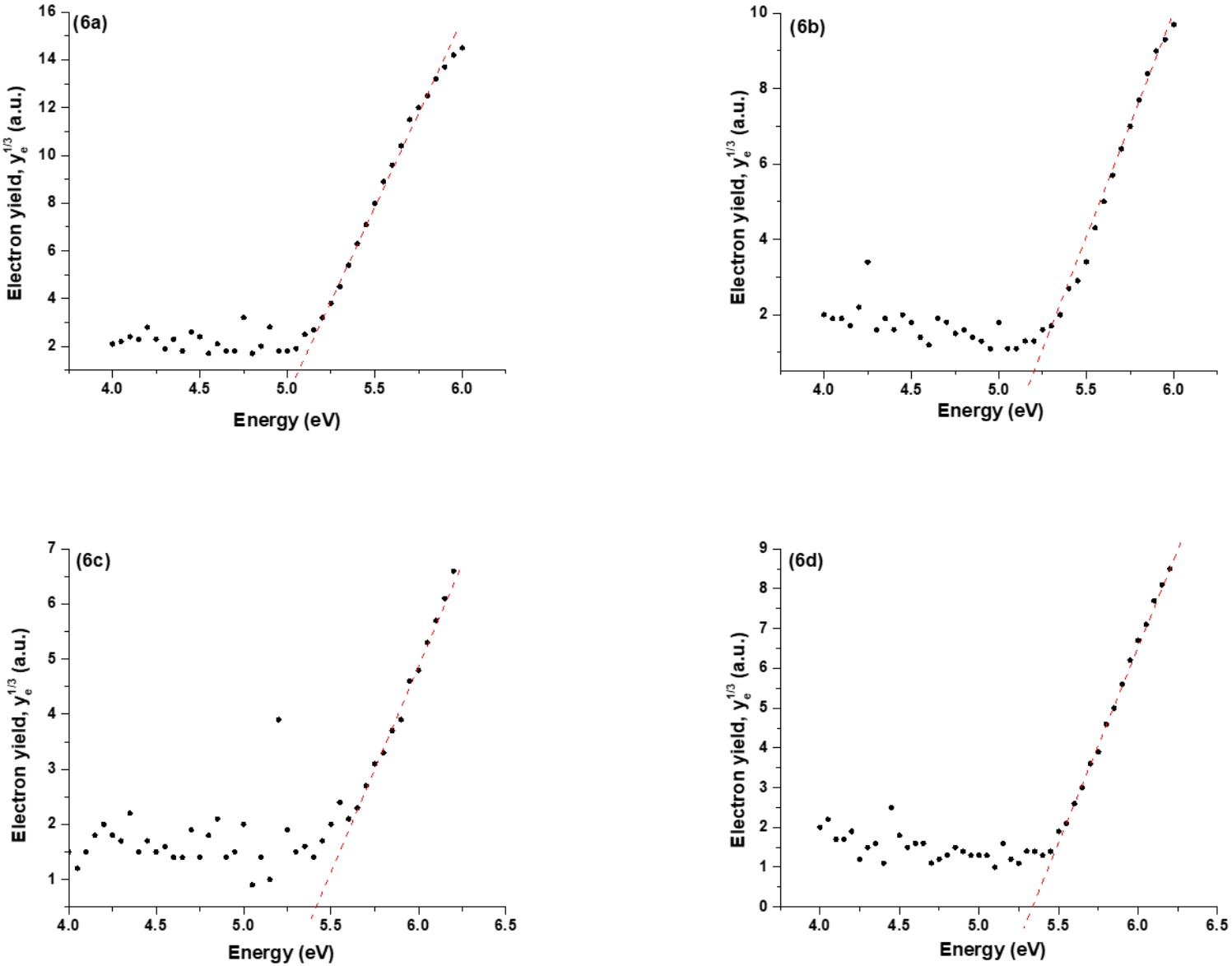


Figure S19. PESA plots of MnPc complexes **(6a-6d)**.

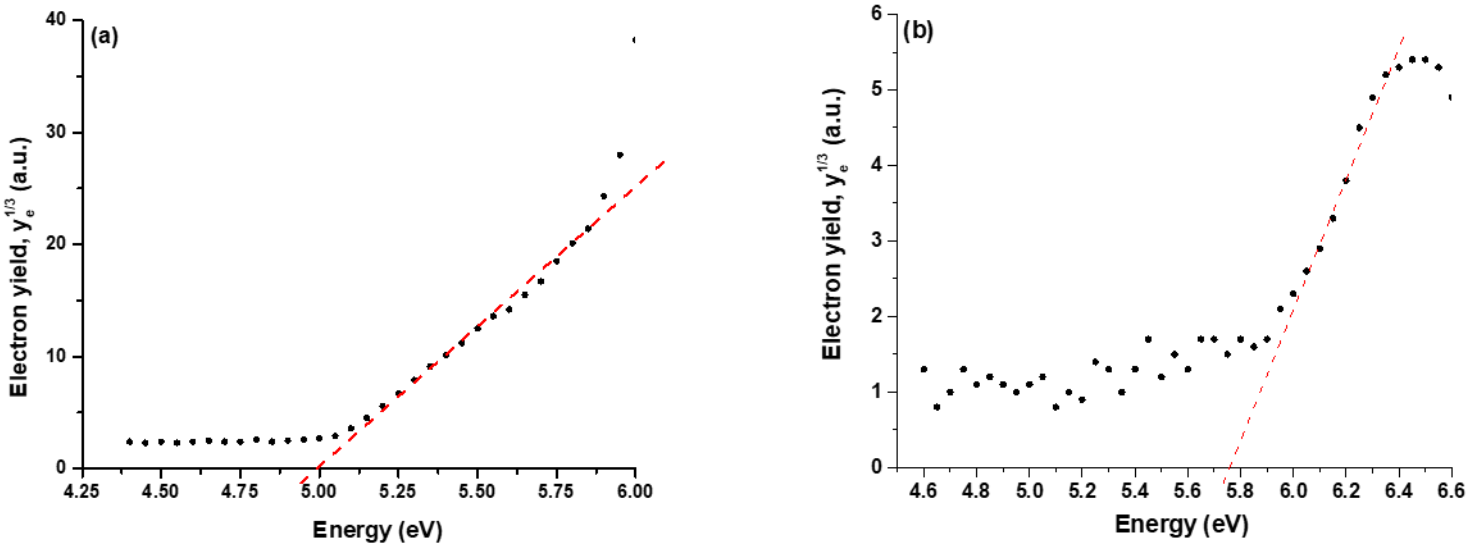


Figure S20. PESA plots of (a) P3HT and (b) $PC_{70}BM$.

(g) DFT Study – Optimised cartesian coordinates

Density functional theory, a computational modelling method was used to investigate the electronic structure of the frontier molecular orbitals of the MPc, i.e. the theoretical HOMO and LUMO values. In this study, B3LYP hybrid DFT functional was coupled with the 6-31+G(d) basis set to calculate the associated energy levels of the modelled MPc complexes. The geometries of all 16 MPcs were optimised prior to extracting HOMO and LUMO information.

Table S4. Optimised cartesian coordinates for MPcs **3a, 4a, 5a** and **6a**.

3a				**4a**				**5a**				**6a**			
C	-3.6328	-2.16701	-0.41138	**C**	-3.59876	-2.15477	-0.3784	**C**	-3.53139	-2.23946	0.01244	**C**	-3.53139	-2.23946	0.01244
C	-4.14681	-0.86278	-0.32497	**C**	-4.11338	-0.8533	-0.28673	**C**	-4.07228	-1.02122	0.20533	**C**	-4.07228	-1.02122	0.20533
C	-5.5213	-0.64083	-0.27428	**C**	-5.49094	-0.63161	-0.22898	**C**	-5.44771	-0.81541	0.18408	**C**	-5.44771	-0.81541	0.18408
C	-6.37156	-1.7455	-0.30951	**C**	-6.3358	-1.73577	-0.26273	**C**	-6.26609	-1.94043	-0.09045	**C**	-6.26609	-1.94043	-0.09045
C	-5.84404	-3.04958	-0.38589	**C**	-5.80588	-3.04289	-0.34434	**C**	-5.67117	-3.21553	-0.32622	**C**	-5.67117	-3.21553	-0.32622
C	-4.46543	-3.27929	-0.43991	**C**	-4.43113	-3.27148	-0.40467	**C**	-4.28134	-3.36554	-0.25289	**C**	-4.28134	-3.36554	-0.25289
C	-2.17278	-2.01351	-0.44934	**C**	-2.1506	-2.0176	-0.4258	**C**	-2.02459	-2.09701	0.13358	**C**	-2.02459	-2.09701	0.13358
C	-2.98191	0.02264	-0.31451	**C**	-2.97061	0.04091	-0.28054	**C**	-2.89818	-0.05297	0.41162	**C**	-2.89818	-0.05297	0.41162
H	-7.44733	-1.60986	-0.28396	**H**	-7.41178	-1.60328	-0.23284	**H**	-7.32889	-1.83001	-0.12109	**H**	-7.32889	-1.83001	-0.12109
H	-4.08055	-4.29104	-0.50504	**H**	-4.04292	-4.28142	-0.4741	**H**	-3.81757	-4.31802	-0.40136	**H**	-3.81757	-4.31802	-0.40136
N	-1.82248	-0.69601	-0.39052	**N**	-1.79924	-0.68517	-0.36735	**N**	-1.74422	-0.79094	0.40626	**N**	-1.74422	-0.79094	0.40626
N	-1.36513	-3.07396	-0.5316	**N**	-1.34652	-3.06126	-0.51586	**N**	-1.21688	-3.09484	-0.00858	**N**	-1.21688	-3.09484	-0.00858
N	-3.11507	1.35059	-0.23851	**N**	-3.09886	1.35348	-0.20349	**N**	-3.02265	1.24673	0.53433	**N**	-3.02265	1.24673	0.53433
C	-2.09959	2.18953	-0.22948	**C**	-2.05267	2.15886	-0.19831	**C**	-2.02672	2.0938	0.42362	**C**	-2.02672	2.0938	0.42362
C	-2.20067	3.63798	-0.14946	**C**	-2.18583	3.60577	-0.11741	**C**	-2.17627	3.62384	0.25715	**C**	-2.17627	3.62384	0.25715
C	-0.88746	4.15686	-0.17075	**C**	-0.88328	4.12115	-0.13812	**C**	-0.9231	4.10503	0.0842	**C**	-0.9231	4.10503	0.0842
C	-3.31994	4.46818	-0.05963	**C**	-3.30885	4.42904	-0.02832	**C**	-3.29642	4.47354	0.26419	**C**	-3.29642	4.47354	0.26419
C	0.02878	3.03835	-0.26357	**C**	0.00932	2.98191	-0.22997	**C**	0.0376	2.9316	0.20322	**C**	0.0376	2.9316	0.20322
C	-0.6709	5.53811	-0.10286	**C**	-0.66037	5.49992	-0.07137	**C**	-0.64962	5.44229	-0.15021	**C**	-0.64962	5.44229	-0.15021
C	-3.08742	5.84133	0.00139	**C**	-3.07663	5.80377	0.03158	**C**	-3.04549	5.8686	0.10171	**C**	-3.04549	5.8686	0.10171
H	-4.32071	4.05455	-0.03558	**H**	-4.3093	4.01449	-0.00355	**H**	-4.28966	4.09129	0.39122	**H**	-4.28966	4.09129	0.39122
C	-1.77522	6.37077	-0.01905	**C**	-1.76633	6.33389	0.01109	**C**	-1.72984	6.33467	-0.13946	**C**	-1.72984	6.33467	-0.13946
H	-1.6642	7.44898	0.03428	**H**	-1.65564	7.41225	0.06364	**H**	-1.56152	7.37747	-0.30875	**H**	-1.56152	7.37747	-0.30875
N	-0.75313	1.9028	-0.29374	**N**	-0.71951	1.80865	-0.26436	**N**	-0.6855	1.80801	0.42056	**N**	-0.6855	1.80801	0.42056

C	-0.04975	-2.99148	-0.5736	**C**	-0.03275	-2.93082	-0.56075	**C**	0.04853	-2.95997	-0.13968	**C**	0.04853	-2.95997	-0.13968
C	0.86644	-4.11008	-0.66564	**C**	0.85986	-4.06899	-0.66703	**C**	0.98688	-4.06568	-0.57714	**C**	0.98688	-4.06568	-0.57714
C	2.17968	-3.59128	-0.68713	**C**	2.16228	-3.55336	-0.68835	**C**	2.22575	-3.52214	-0.70438	**C**	2.22575	-3.52214	-0.70438
C	0.64972	-5.4913	-0.73392	**C**	0.63663	-5.44701	-0.74706	**C**	0.71226	-5.39772	-0.83522	**C**	0.71226	-5.39772	-0.83522
C	2.0786	-2.14278	-0.60808	**C**	2.02903	-2.1073	-0.59301	**C**	2.13137	-2.02592	-0.30804	**C**	2.13137	-2.02592	-0.30804
C	3.29887	-4.42158	-0.77741	**C**	3.28502	-4.37561	-0.79131	**C**	3.31682	-4.2823	-1.1374	**C**	3.31682	-4.2823	-1.1374
C	1.75391	-6.32403	-0.81804	**C**	1.74226	-6.27999	-0.84334	**C**	1.77626	-6.19759	-1.28103	**C**	1.77626	-6.19759	-1.28103
C	3.06617	-5.79467	-0.83868	**C**	3.0525	-5.74961	-0.86479	**C**	3.07168	-5.64623	-1.44545	**C**	3.07168	-5.64623	-1.44545
H	4.29966	-4.00802	-0.80217	**H**	4.28533	-3.96076	-0.81667	**H**	4.29168	-3.85132	-1.23476	**H**	4.29168	-3.85132	-1.23476
N	0.73214	-1.85602	-0.5432	**N**	0.69663	-1.75763	-0.51764	**N**	0.8483	-1.74543	0.0596	**N**	0.8483	-1.74543	0.0596
N	1.34407	3.12095	-0.30779	**N**	1.32327	3.11236	-0.27061	**N**	1.31424	3.0566	0.12866	**N**	1.31424	3.0566	0.12866
N	3.09384	-1.30361	-0.60203	**N**	3.0752	-1.30217	-0.58465	**N**	3.12679	-1.22171	-0.3286	**N**	3.12679	-1.22171	-0.3286
C	2.96046	0.02445	-0.52819	**C**	2.94674	0.00985	-0.50413	**C**	2.99745	0.04164	-0.15354	**C**	2.99745	0.04164	-0.15354
C	4.12505	0.91027	-0.52815	**C**	4.08931	0.90424	-0.50115	**C**	4.14998	1.0437	-0.32649	**C**	4.14998	1.0437	-0.32649
C	3.61134	2.21456	-0.44172	**C**	3.57523	2.20567	-0.40943	**C**	3.60947	2.26349	-0.20155	**C**	3.60947	2.26349	-0.20155
C	5.4989	0.68837	-0.59637	**C**	5.4663	0.68229	-0.57338	**C**	5.50883	0.86137	-0.57382	**C**	5.50883	0.86137	-0.57382
C	2.15169	2.06066	-0.39262	**C**	2.12716	2.06898	-0.358	**C**	2.13239	2.07187	0.07438	**C**	2.13239	2.07187	0.07438
C	4.44462	3.32664	-0.41136	**C**	4.40862	3.3219	-0.37638	**C**	4.33565	3.43017	-0.33077	**C**	4.33565	3.43017	-0.33077
C	6.34884	1.79339	-0.57421	**C**	6.31116	1.78643	-0.54834	**C**	6.3057	2.02837	-0.7116	**C**	6.3057	2.02837	-0.7116
C	5.8224	3.09662	-0.477	**C**	5.78263	3.09266	-0.44538	**C**	5.7053	3.3178	-0.60415	**C**	5.7053	3.3178	-0.60415
H	7.42346	1.66	-0.6369	**H**	7.38597	1.65611	-0.61335	**H**	7.3546	1.93958	-0.89865	**H**	7.3546	1.93958	-0.89865
N	1.80137	0.74289	-0.44622	**N**	1.77503	0.73597	-0.41489	**N**	1.8706	0.74116	0.19505	**N**	1.8706	0.74116	0.19505
H	4.06021	4.33838	-0.34307	**H**	4.02099	4.33182	-0.30364	**H**	3.86929	4.38657	-0.22786	**H**	3.86929	4.38657	-0.22786
H	-0.3581	-5.89346	-0.71867	**H**	-0.37111	-5.84961	-0.73157	**H**	-0.27289	-5.79941	-0.70182	**H**	-0.27289	-5.79941	-0.70182
H	-5.92052	0.36724	-0.2181	**H**	-5.8893	0.37636	-0.16965	**H**	-5.87036	0.15113	0.36388	**H**	-5.87036	0.15113	0.36388
H	0.33685	5.94043	-0.11865	**H**	0.34744	5.9024	-0.08668	**H**	0.34824	5.78215	-0.3271	**H**	0.34824	5.78215	-0.3271
H	5.89676	-0.31883	-0.67378	**H**	5.86295	-0.32474	-0.65555	**H**	5.93315	-0.11679	-0.65647	**H**	5.93315	-0.11679	-0.65647
C	-5.40738	6.43818	-0.11033	**C**	-5.39534	6.40266	-0.09856	**C**	-5.38692	6.42927	-0.15782	**C**	-5.38692	6.42927	-0.15782
C	-6.31645	6.55875	0.93392	**C**	-6.32382	6.53908	0.92683	**C**	-6.46182	6.95492	0.56982	**C**	-6.46182	6.95492	0.56982
C	-5.84477	6.07053	-1.38418	**C**	-5.81179	6.0215	-1.37581	**C**	-5.61763	5.51704	-1.19301	**C**	-5.61763	5.51704	-1.19301
C	-7.67168	6.30788	0.703	**C**	-7.67571	6.29076	0.67387	**C**	-7.76969	6.58053	0.26157	**C**	-7.76969	6.58053	0.26157
H	-5.96126	6.85404	1.91634	**H**	-5.98547	6.8443	1.91217	**H**	-6.27762	7.6475	1.36706	**H**	-6.27762	7.6475	1.36706
C	-7.19732	5.8173	-1.59319	**C**	-7.16094	5.77072	-1.6068	**C**	-6.93637	5.14564	-1.50963	**C**	-6.93637	5.14564	-1.50963
H	-5.13144	5.98961	-2.1987	**H**	-5.08398	5.92746	-2.17598	**H**	-4.79547	5.10827	-1.74222	**H**	-4.79547	5.10827	-1.74222

C	-8.14549	5.92833	-0.55981	**C**	-8.12774	5.89764	-0.59287	**C**	-8.01195	5.68164	-0.77822	**C**	-8.01195	5.68164	-0.77822
H	-8.35802	6.41246	1.53566	**H**	-8.3768	6.40788	1.49254	**H**	-8.58992	6.98145	0.82317	**H**	-8.58992	6.98145	0.82317
H	-7.51742	5.53299	-2.59151	**H**	-7.46346	5.47545	-2.60751	**H**	-7.12155	4.45708	-2.30731	**H**	-7.12155	4.45708	-2.30731
O	-4.08131	6.78094	0.12414	**O**	-4.07394	6.7425	0.1567	**O**	-4.07443	6.86339	0.19077	**O**	-4.07443	6.86339	0.19077
C	-7.88089	-4.22051	0.13229	**C**	-7.84321	-4.21154	0.17806	**C**	-7.7234	-4.34566	-0.00252	**C**	-7.7234	-4.34566	-0.00252
C	-8.07977	-3.81262	1.45032	**C**	-8.03727	-3.80798	1.49799	**C**	-7.91149	-3.62889	1.18592	**C**	-7.91149	-3.62889	1.18592
C	-8.93087	-4.79674	-0.58359	**C**	-8.89571	-4.78378	-0.53711	**C**	-8.7855	-5.05853	-0.56986	**C**	-8.7855	-5.05853	-0.56986
C	-9.3362	-3.97332	2.03893	**C**	-9.29269	-3.96844	2.08929	**C**	-9.1629	-3.64798	1.81984	**C**	-9.1629	-3.64798	1.81984
H	-7.26135	-3.37701	2.01472	**H**	-7.2164	-3.37638	2.06203	**H**	-7.10243	-3.07082	1.60881	**H**	-7.10243	-3.07082	1.60881
C	-10.1727	-4.95623	0.02414	**C**	-10.136	-4.94356	0.07335	**C**	-10.0296	-5.08542	0.0654	**C**	-10.0296	-5.08542	0.0654
H	-8.75883	-5.11674	-1.60659	**H**	-8.72679	-5.10047	-1.56166	**H**	-8.64344	-5.58595	-1.48933	**H**	-8.64344	-5.58595	-1.48933
C	-10.4123	-4.54653	1.34737	**C**	-10.3715	-4.5377	1.39846	**C**	-10.2194	-4.38609	1.2629	**C**	-10.2194	-4.38609	1.2629
H	-9.45965	-3.64645	3.06546	**H**	-9.41315	-3.64477	3.11716	**H**	-9.31082	-3.10221	2.72788	**H**	-9.31082	-3.10221	2.72788
H	-10.9731	-5.40836	-0.55495	**H**	-10.9384	-5.39262	-0.5051	**H**	-10.8379	-5.64173	-0.36497	**H**	-10.8379	-5.64173	-0.36497
O	-6.64751	-4.16492	-0.49253	**O**	-6.61193	-4.15516	-0.45177	**O**	-6.45085	-4.36782	-0.64436	**O**	-6.45085	-4.36782	-0.64436
C	7.8863	4.21057	0.04676	**C**	7.84867	4.19905	0.08328	**C**	7.75516	4.40932	-0.18513	**C**	7.75516	4.40932	-0.18513
C	8.14013	3.6841	1.31229	**C**	8.09704	3.67456	1.35048	**C**	7.97167	3.54254	0.89305	**C**	7.97167	3.54254	0.89305
C	8.90933	4.84054	-0.66264	**C**	8.87582	4.82206	-0.6262	**C**	8.80687	5.18223	-0.69044	**C**	8.80687	5.18223	-0.69044
C	9.42348	3.78213	1.85439	**C**	9.3801	3.76758	1.8946	**C**	9.23953	3.47268	1.48532	**C**	9.23953	3.47268	1.48532
H	7.34318	3.20493	1.8721	**H**	7.29641	3.20152	1.91038	**H**	7.17055	2.93722	1.26561	**H**	7.17055	2.93722	1.26561
C	10.17957	4.93488	-0.10141	**C**	10.1454	4.91165	-0.06294	**C**	10.07151	5.1173	-0.09552	**C**	10.07151	5.1173	-0.09552
H	8.69502	5.25211	-1.64409	**H**	8.66518	5.23218	-1.60905	**H**	8.64158	5.82506	-1.52994	**H**	8.64158	5.82506	-1.52994
C	10.47403	4.40641	1.16766	**C**	10.43486	4.38502	1.20804	**C**	10.28618	4.27076	0.99867	**C**	10.28618	4.27076	0.99867
H	9.58917	3.364	2.84111	**H**	9.54209	3.35134	2.8827	**H**	9.408	2.81272	2.31019	**H**	9.408	2.81272	2.31019
H	10.9581	5.43	-0.67523	**H**	10.92741	5.40153	-0.63647	**H**	10.87399	5.71434	-0.4753	**H**	10.87399	5.71434	-0.4753
O	6.62458	4.21756	-0.52171	**O**	6.58775	4.21043	-0.48819	**O**	6.46088	4.52015	-0.76896	**O**	6.46088	4.52015	-0.76896
C	-11.8069	-4.73566	1.97093	**C**	-11.765	-4.72677	2.0243	**C**	-11.5912	-4.43295	1.95907	**C**	-11.5912	-4.43295	1.95907
C	-12.1805	-6.23708	1.9583	**C**	-12.138	-6.22836	2.0134	**C**	-12.2641	-5.79119	1.67401	**C**	-12.2641	-5.79119	1.67401
H	-13.1766	-6.38691	2.39262	**H**	-13.1332	-6.37824	2.44979	**H**	-13.2189	-5.82625	2.15641	**H**	-13.2189	-5.82625	2.15641
H	-12.1968	-6.6456	0.94233	**H**	-12.1562	-6.63753	0.99771	**H**	-12.3934	-5.91142	0.6188	**H**	-12.3934	-5.91142	0.6188
H	-11.4628	-6.8242	2.54255	**H**	-11.419	-6.81485	2.59661	**H**	-11.6462	-6.58062	2.05008	**H**	-11.6462	-6.58062	2.05008
C	-12.8505	-3.94228	1.14882	**C**	-12.8101	-3.93435	1.20303	**C**	-12.4756	-3.29347	1.41866	**C**	-12.4756	-3.29347	1.41866
H	-13.8527	-4.07198	1.5756	**H**	-13.8115	-4.06396	1.63152	**H**	-13.4313	-3.3226	1.89932	**H**	-13.4313	-3.3226	1.89932
H	-12.617	-2.87139	1.14885	**H**	-12.5769	-2.8634	1.20178	**H**	-12.0054	-2.35257	1.61715	**H**	-12.0054	-2.35257	1.61715

H	-12.8868	-4.27572	0.10633	**H**	-12.8481	-4.26875	0.16088	**H**	-12.604	-3.41222	0.36286	**H**	-12.604	-3.41222	0.36286
C	-11.8685	-4.24029	3.42848	**C**	-11.8245	-4.23011	3.48147	**C**	-11.4049	-4.26213	3.47872	**C**	-11.4049	-4.26213	3.47872
H	-11.1684	-4.78284	4.07398	**H**	-11.1225	-4.77122	4.12618	**H**	-10.7887	-5.05181	3.85449	**H**	-10.7887	-5.05181	3.85449
H	-11.6469	-3.16965	3.50652	**H**	-11.6041	-3.15909	3.55805	**H**	-10.937	-3.31982	3.67678	**H**	-10.937	-3.31982	3.67678
H	-12.8761	-4.39775	3.8292	**H**	-12.8311	-4.38844	3.88422	**H**	-12.3597	-4.29411	3.96173	**H**	-12.3597	-4.29411	3.96173
C	-9.63047	5.64014	-0.84603	**C**	-9.60792	5.61025	-0.90343	**C**	-9.47076	5.30339	-1.09633	**C**	-9.47076	5.30339	-1.09633
C	-9.78558	4.18516	-1.3492	**C**	-9.75781	4.1508	-1.39503	**C**	-9.53234	3.87112	-1.6618	**C**	-9.53234	3.87112	-1.6618
H	-10.8386	3.96671	-1.56464	**H**	-10.8073	3.93265	-1.62767	**H**	-10.5499	3.61558	-1.876	**H**	-10.5499	3.61558	-1.876
H	-9.21476	4.00667	-2.26664	**H**	-9.1705	3.96189	-2.29989	**H**	-8.95458	3.81405	-2.56083	**H**	-8.95458	3.81405	-2.56083
H	-9.43738	3.47018	-0.59502	**H**	-9.42526	3.44265	-0.62742	**H**	-9.13728	3.18581	-0.9403	**H**	-9.13728	3.18581	-0.9403
C	-10.1452	6.61506	-1.93183	**C**	-10.1005	6.57572	-2.00782	**C**	-10.0447	6.29517	-2.13262	**C**	-10.0447	6.29517	-2.13262
H	-11.2028	6.42091	-2.14796	**H**	-11.154	6.38068	-2.2431	**H**	-11.0612	6.03952	-2.3478	**H**	-11.0612	6.03952	-2.3478
H	-10.051	7.65548	-1.60058	**H**	-10.0117	7.61899	-1.68412	**H**	-10.0032	7.28927	-1.73804	**H**	-10.0032	7.28927	-1.73804
H	-9.58991	6.51167	-2.86996	**H**	-9.52694	6.4636	-2.93387	**H**	-9.46754	6.24524	-3.03337	**H**	-9.46754	6.24524	-3.03337
C	-10.5106	5.81059	0.40675	**C**	-10.5102	5.79499	0.3314	**C**	-10.3009	5.37459	0.20094	**C**	-10.3009	5.37459	0.20094
H	-10.2145	5.12618	1.20996	**H**	-10.2295	5.11853	1.1468	**H**	-9.90288	4.68448	0.91581	**H**	-9.90288	4.68448	0.91581
H	-10.4721	6.83409	0.79686	**H**	-10.4766	6.82242	0.7114	**H**	-10.2567	6.36667	0.59985	**H**	-10.2567	6.36667	0.59985
H	-11.5548	5.59272	0.15622	**H**	-11.5501	5.57624	0.06436	**H**	-11.3189	5.12104	-0.01125	**H**	-11.3189	5.12104	-0.01125
C	11.89741	4.52752	1.74133	**C**	11.8578	4.50112	1.78391	**C**	11.67277	4.21817	1.66746	**C**	11.67277	4.21817	1.66746
C	12.28814	6.02113	1.84557	**C**	12.25647	5.9931	1.88177	**C**	12.35441	5.59627	1.53813	**C**	12.35441	5.59627	1.53813
H	13.30431	6.12371	2.24581	**H**	13.27213	6.09192	2.28416	**H**	13.31825	5.56526	2.00209	**H**	13.31825	5.56526	2.00209
H	12.26388	6.51852	0.87027	**H**	12.23765	6.48588	0.904	**H**	12.46514	5.84406	0.50297	**H**	12.46514	5.84406	0.50297
H	11.60399	6.55926	2.51149	**H**	11.57365	6.53831	2.54328	**H**	11.75115	6.33834	2.01963	**H**	11.75115	6.33834	2.01963
C	12.89316	3.80297	0.80452	**C**	12.85125	3.76647	0.85247	**C**	12.53431	3.14561	0.97462	**C**	12.53431	3.14561	0.97462
H	13.91555	3.88873	1.19277	**H**	13.87328	3.84818	1.24245	**H**	13.49884	3.10666	1.43626	**H**	13.49884	3.10666	1.43626
H	12.64883	2.7377	0.72181	**H**	12.60103	2.70224	0.77422	**H**	12.05678	2.19191	1.0656	**H**	12.05678	2.19191	1.0656
H	12.88407	4.22647	-0.20537	**H**	12.8467	4.18537	-0.15938	**H**	12.64468	3.39167	-0.06104	**H**	12.64468	3.39167	-0.06104
C	12.01807	3.90264	3.14418	**C**	11.97212	3.88237	3.18997	**C**	11.51112	3.86083	3.15763	**C**	11.51112	3.86083	3.15763
H	11.35728	4.3934	3.86787	**H**	11.31202	4.37982	3.90972	**H**	10.90975	4.60273	3.63957	**H**	10.90975	4.60273	3.63957
H	11.78267	2.83223	3.13586	**H**	11.73165	2.81306	3.18624	**H**	11.03655	2.90523	3.24493	**H**	11.03655	2.90523	3.24493
H	13.04557	4.01104	3.50915	**H**	12.99924	3.9876	3.55687	**H**	12.47391	3.82403	3.62382	**H**	12.47391	3.82403	3.62382
O	4.05985	-6.73447	-0.96161	**O**	4.04879	-6.68758	-1.00387	**O**	4.09999	-6.5089	-1.93464	**O**	4.09999	-6.5089	-1.93464
C	5.38643	-6.39077	-0.7314	**C**	5.37363	-6.35035	-0.76303	**C**	5.38298	-6.16813	-1.4214	**C**	5.38298	-6.16813	-1.4214
C	5.82798	-6.02713	0.54215	**C**	5.80921	-5.98121	0.51129	**C**	5.51389	-5.51476	-0.18864	**C**	5.51389	-5.51476	-0.18864

C	6.29177	-6.50631	-1.77944	**C**	6.28688	-6.47803	-1.80323	**C**	6.51503	-6.50094	-2.16685	**C**	6.51503	-6.50094	-2.16685
C	7.18099	-5.77309	0.74719	**C**	7.16238	-5.73429	0.72432	**C**	6.79387	-5.21543	0.30836	**C**	6.79387	-5.21543	0.30836
H	5.11739	-5.95015	1.35946	**H**	5.09339	-5.89375	1.32293	**H**	4.63947	-5.24962	0.37207	**H**	4.63947	-5.24962	0.37207
C	7.64753	-6.25462	-1.55255	**C**	7.64255	-6.23382	-1.56844	**C**	7.78479	-6.22892	-1.66424	**C**	7.78479	-6.22892	-1.66424
H	5.93339	-6.79836	-2.76166	**H**	5.93355	-6.77384	-2.78617	**H**	6.40755	-6.97167	-3.1207	**H**	6.40755	-6.97167	-3.1207
C	8.12549	-5.87929	-0.29004	**C**	8.11399	-5.85324	-0.3051	**C**	7.92927	-5.59362	-0.42738	**C**	7.92927	-5.59362	-0.42738
H	7.5045	-5.49215	1.74537	**H**	7.48038	-5.44867	1.72302	**H**	6.9038	-4.7031	1.24339	**H**	6.9038	-4.7031	1.24339
H	8.33094	-6.35516	-2.38809	**H**	8.33107	-6.34425	-2.39857	**H**	8.64937	-6.50627	-2.22844	**H**	8.64937	-6.50627	-2.22844
C	9.61122	-5.59072	-0.0081	**C**	9.59939	-5.57127	-0.01451	**C**	9.34337	-5.32538	0.10997	**C**	9.34337	-5.32538	0.10997
C	9.76682	-4.13719	0.49909	**C**	9.75921	-4.11661	0.48791	**C**	9.35437	-4.02667	0.93181	**C**	9.35437	-4.02667	0.93181
H	9.4153	-3.42013	-0.25155	**H**	9.41648	-3.40108	-0.26824	**H**	9.05118	-3.21023	0.31047	**H**	9.05118	-3.21023	0.31047
H	9.19906	-3.96226	1.41915	**H**	9.18561	-3.93531	1.40308	**H**	8.67738	-4.11983	1.75508	**H**	8.67738	-4.11983	1.75508
H	10.82043	-3.9185	0.71142	**H**	10.81243	-3.9023	0.70684	**H**	10.34274	-3.84589	1.30161	**H**	10.34274	-3.84589	1.30161
C	10.13045	-6.56858	1.07288	**C**	10.1069	-6.54694	1.07387	**C**	9.77046	-6.50249	1.0071	**C**	9.77046	-6.50249	1.0071
H	10.03573	-7.60804	0.73883	**H**	10.00978	-7.5872	0.74306	**H**	9.75774	-7.40911	0.43932	**H**	9.75774	-7.40911	0.43932
H	11.18879	-6.37444	1.28571	**H**	11.1646	-6.35669	1.29352	**H**	10.75755	-6.32968	1.3807	**H**	10.75755	-6.32968	1.3807
H	9.57854	-6.46838	2.01335	**H**	9.54862	-6.44068	2.00986	**H**	9.08825	-6.58664	1.82867	**H**	9.08825	-6.58664	1.82867
C	10.48719	-5.75651	-1.26442	**C**	10.48349	-5.74641	-1.26383	**C**	10.32059	-5.19166	-1.07824	**C**	10.32059	-5.19166	-1.07824
H	10.44811	-6.77878	-1.65767	**H**	10.44102	-6.76976	-1.65377	**H**	10.31298	-6.09722	-1.65064	**H**	10.31298	-6.09722	-1.65064
H	10.18796	-5.06976	-2.06444	**H**	10.1938	-5.06084	-2.06833	**H**	10.01663	-4.37552	-1.69923	**H**	10.01663	-4.37552	-1.69923
H	11.53212	-5.5387	-1.01679	**H**	11.52789	-5.53379	-1.00946	**H**	11.30996	-5.01215	-0.71082	**H**	11.30996	-5.01215	-0.71082
H	1.6428	-7.4022	-0.87193	**H**	1.63141	-7.35773	-0.90695	**H**	1.60731	-7.22972	-1.50023	**H**	1.60731	-7.22972	-1.50023
Co	-0.12659	-0.02302	0.00143	**Ni**	-0.01149	0.02564	-0.39099	**Ti**	0.07312	-0.01638	0.7821	**Mn**	0.07312	-0.01638	0.7821
								O	0.03409	-0.05736	2.52112	**Cl**	0.03048	-0.06115	2.6819

Table S5. Optimised cartesian coordinates for MPcs **3b, 4b, 5b** and **6b**.

3b				**4b**				**5b**				**6b**			
C	-3.6271	-2.12978	-0.38012	**C**	-3.57393	-2.18102	-0.31555	**C**	-3.59773	-2.33726	-0.00513	**C**	-3.44148	-2.13234	-0.03228
C	-4.12648	-0.89262	-0.29333	**C**	-4.09289	-0.87529	-0.32599	**C**	-4.10984	-1.07837	0.05195	**C**	-3.92635	-0.89264	0.01511
C	-5.4964	-0.64296	-0.22461	**C**	-5.47116	-0.65447	-0.33089	**C**	-5.47185	-0.85668	0.2556	**C**	-5.28206	-0.62834	-0.20699

C	-6.36508	-1.76465	-0.27119	**C**	-6.3167	-1.76116	-0.31985	**C**	-6.31949	-1.99399	0.33049	**C**	-6.12935	-1.72894	-0.49554
C	-5.82083	-3.07802	-0.38812	**C**	-5.78353	-3.06749	-0.29542	**C**	-5.77334	-3.3074	0.22174	**C**	-5.58733	-3.04148	-0.57737
C	-4.42835	-3.25863	-0.41915	**C**	-4.40465	-3.29744	-0.2969	**C**	-4.37839	-3.47875	0.1043	**C**	-4.21777	-3.24668	-0.33403
C	-2.10539	-2.00513	-0.42815	**C**	-2.13029	-2.04169	-0.32009	**C**	-2.10565	-2.18103	-0.22276	**C**	-1.9724	-2.01096	0.28821
C	-2.92037	0.05737	-0.28339	**C**	-2.95416	0.01311	-0.33408	**C**	-3.04782	-0.16177	-0.14753	**C**	-2.85858	-0.0205	0.30535
H	-7.42504	-1.62049	-0.21619	**H**	-7.3929	-1.62802	-0.33796	**H**	-7.37236	-1.86428	0.46544	**H**	-7.17642	-1.57157	-0.65638
H	-3.99954	-4.23774	-0.47194	**H**	-4.0161	-4.30961	-0.28503	**H**	-3.93786	-4.45399	0.08701	**H**	-3.78884	-4.22486	-0.38356
N	-1.75727	-0.67743	-0.37839	**N**	-1.77596	-0.70873	-0.32962	**N**	-1.87973	-0.8571	-0.2522	**N**	-1.6749	-0.7063	0.51793
N	-1.34442	-3.03198	-0.5026	**N**	-1.31957	-3.1041	-0.31984	**N**	-1.20361	-3.17511	-0.38453	**N**	-1.19288	-3.03499	0.30845
N	-3.04084	1.32445	-0.19918	**N**	-3.0928	1.34387	-0.34382	**N**	-3.19074	1.17652	-0.27859	**N**	-3.04443	1.26205	0.33632
C	-2.03968	2.11553	-0.18873	**C**	-2.04878	2.12765	-0.34416	**C**	-2.19704	2.02337	-0.29329	**C**	-2.09174	2.05694	0.50379
C	-2.17564	3.63475	-0.09685	**C**	-2.18207	3.59006	-0.35165	**C**	-2.30256	3.50059	-0.70397	**C**	-2.19788	3.50859	0.01702
C	-0.92563	4.12656	-0.12724	**C**	-0.88538	4.10495	-0.34194	**C**	-1.05528	4.02968	-0.67289	**C**	-0.96133	4.01191	0.02145
C	-3.30963	4.46075	0.00257	**C**	-3.30489	4.40662	-0.37269	**C**	-3.41324	4.26147	-1.06904	**C**	-3.3043	4.25727	-0.40852
C	0.01956	2.93644	-0.22421	**C**	0.02047	2.95788	-0.33002	**C**	-0.07591	2.9424	-0.24483	**C**	-0.01337	2.92047	0.48073
C	-0.65492	5.4857	-0.07979	**C**	-0.66204	5.47952	-0.35266	**C**	-0.79245	5.35234	-1.00465	**C**	-0.67651	5.311	-0.37163
C	-3.078	5.86171	0.07134	**C**	-3.07671	5.79106	-0.37582	**C**	-3.19213	5.61965	-1.40121	**C**	-3.0616	5.58613	-0.83603
H	-4.30015	4.05149	0.01944	**H**	-4.30532	3.99098	-0.39389	**H**	-4.39324	3.83643	-1.09636	**H**	-4.29198	3.84389	-0.41421
C	-1.75348	6.35991	0.01203	**C**	-1.77355	6.32074	-0.36694	**C**	-1.88108	6.15958	-1.37314	**C**	-1.74714	6.10996	-0.80251
H	-1.58786	7.41688	0.03992	**H**	-1.66198	7.40014	-0.37398	**H**	-1.7192	7.18484	-1.63164	**H**	-1.57003	7.11768	-1.10821
N	-0.7126	1.78332	-0.25696	**N**	-0.70609	1.77027	-0.33322	**N**	-0.80543	1.71541	0.1332	**N**	-0.75164	1.7969	1.14867
C	-0.08097	-2.92539	-0.54774	**C**	-0.02048	-2.95844	-0.3292	**C**	0.09272	-3.00559	-0.33877	**C**	0.03208	-2.91233	0.49611
C	0.88832	-4.09709	-0.66165	**C**	0.88537	-4.1055	-0.34053	**C**	1.11349	-4.06943	-0.73401	**C**	0.96997	-4.01041	0.0243
C	2.1454	-3.58549	-0.69268	**C**	2.18206	-3.59061	-0.35011	**C**	2.35366	-3.50912	-0.71126	**C**	2.20535	-3.50731	-0.00063
C	0.62872	-5.45231	-0.72944	**C**	0.66206	-5.48008	-0.35081	**C**	0.90047	-5.39675	-1.08457	**C**	0.67622	-5.31277	-0.35749
C	2.02499	-2.0468	-0.58559	**C**	2.04877	-2.1282	-0.34312	**C**	2.20453	-2.03121	-0.29933	**C**	2.11173	-2.05195	0.47564
C	3.27782	-4.40297	-0.81008	**C**	3.3049	-4.40717	-0.37063	**C**	3.49844	-4.24306	-1.04265	**C**	3.30362	-4.25885	-0.43418
C	1.72842	-6.31086	-0.84046	**C**	1.77357	-6.3213	-0.36456	**C**	2.02319	-6.17337	-1.41879	**C**	1.74057	-6.11873	-0.79333
C	3.04801	-5.80084	-0.8981	**C**	3.07674	-5.79161	-0.37336	**C**	3.31923	-5.60252	-1.4022	**C**	3.05644	-5.59509	-0.84203

H	4.2613	-3.98764	-0.83502	**H**	4.30532	-3.99151	-0.39172	**H**	4.47173	-3.79507	-1.02605	**H**	4.28778	-3.84102	-0.46047
N	0.70766	-1.69227	-0.50764	**N**	0.70607	-1.77083	-0.33265	**N**	0.79904	-1.78173	0.12372	**N**	0.78447	-1.78568	1.14384
N	1.29459	3.05364	-0.26698	**N**	1.31956	3.10355	-0.32045	**N**	1.17509	3.112	-0.21099	**N**	1.21474	3.04533	0.27454
N	3.03099	-1.26911	-0.57796	**N**	3.09279	-1.34443	-0.34277	**N**	3.16407	-1.17923	-0.32294	**N**	3.06931	-1.25728	0.28983
C	2.90757	0.00081	-0.50951	**C**	2.95415	-0.01366	-0.33349	**C**	2.96857	0.12657	-0.18344	**C**	2.89048	0.03138	0.27467
C	4.1024	0.94997	-0.50331	**C**	4.09287	0.87474	-0.32553	**C**	4.02344	1.04616	0.01689	**C**	3.95833	0.90582	-0.01184
C	3.60199	2.18665	-0.41555	**C**	3.57391	2.18047	-0.31557	**C**	3.49474	2.28006	0.05722	**C**	3.47094	2.14481	-0.06327
C	5.47498	0.69653	-0.5654	**C**	5.47114	0.65391	-0.33015	**C**	5.39755	0.83971	0.15004	**C**	5.3088	0.64313	-0.22762
C	2.08478	2.05318	-0.36322	**C**	2.13028	2.04114	-0.32026	**C**	2.01069	2.10889	-0.12464	**C**	2.00246	2.02253	0.26015
C	4.40262	3.31396	-0.39065	**C**	4.40463	3.2969	-0.29715	**C**	4.24825	3.43163	0.21174	**C**	4.23705	3.2577	-0.37166
C	6.34487	1.81882	-0.55236	**C**	6.31668	1.7606	-0.31933	**C**	6.22528	1.98782	0.25823	**C**	6.15219	1.74122	-0.51905
C	5.79806	3.13397	-0.48379	**C**	5.78351	3.06694	-0.29539	**C**	5.6463	3.28753	0.25937	**C**	5.60785	3.05285	-0.60708
H	7.40372	1.6738	-0.59319	**H**	7.39289	1.62746	-0.33722	**H**	7.28668	1.8773	0.33594	**H**	7.19693	1.58334	-0.67791
N	1.75276	0.72967	-0.4344	**N**	1.77594	0.70818	-0.32938	**N**	1.75947	0.7877	-0.23704	**N**	1.71084	0.71909	0.50121
H	3.97818	4.28739	-0.30377	**H**	4.01609	4.30907	-0.28565	**H**	3.78522	4.39554	0.27664	**H**	3.79744	4.23251	-0.42799
H	-0.37167	-5.82652	-0.70437	**H**	-0.34623	-5.88136	-0.34507	**H**	-0.08244	-5.8146	-1.09833	**H**	-0.32571	-5.69044	-0.32138
H	-5.87045	0.35342	-0.14397	**H**	-5.8724	0.35388	-0.35204	**H**	-5.86401	0.13508	0.34488	**H**	-5.667	0.3684	-0.16523
H	0.34639	5.85811	-0.11285	**H**	0.34625	5.88078	-0.34683	**H**	0.20417	5.74256	-0.98068	**H**	0.32381	5.69099	-0.34943
H	5.85588	-0.30499	-0.62395	**H**	5.87238	-0.35445	-0.35092	**H**	5.81286	-0.14565	0.1648	**H**	5.693	-0.35381	-0.17211
O	-4.12332	6.8389	0.20792	**O**	-4.08791	6.71944	-0.44129	**O**	-4.27705	6.47332	-1.76604	**O**	-4.11507	6.42951	-1.31566
O	-6.63584	-4.25595	-0.49256	**O**	-6.58254	-4.18941	-0.33866	**O**	-6.60757	-4.47672	0.20805	**O**	-6.41012	-4.16913	-0.9081
O	6.61023	4.3145	-0.52063	**O**	6.58255	4.18884	-0.33884	**O**	6.45768	4.46762	0.28876	**O**	6.4326	4.17523	-0.93978
O	4.09401	-6.76994	-1.05406	**O**	4.08791	-6.72006	-0.43815	**O**	4.43136	-6.43001	-1.75531	**O**	4.11028	-6.44357	-1.31739
H	1.57173	-7.36593	-0.8864	**H**	1.66201	-7.4007	-0.37127	**H**	1.89944	-7.20293	-1.68647	**H**	1.55737	-7.13122	-1.09118
Co	-0.00624	0.04537	-0.37723	**C**	-7.84988	-4.17449	0.21751	**C**	-7.93408	-4.26065	0.70945	**C**	-7.67564	-4.11265	-0.24154
C	-7.88405	-4.21902	0.2078	**C**	-8.87849	-4.7201	-0.51448	**C**	-8.95439	-4.92843	0.11217	**C**	-8.76367	-4.69496	-0.81199
C	-8.95648	-4.932	-0.34113	**C**	-8.06052	-3.70285	1.53889	**C**	-8.19238	-3.38853	1.78236	**C**	-7.78168	-3.47046	0.99957
C	-8.05148	-3.51449	1.4089	**C**	-10.1806	-4.81955	0.04288	**C**	-10.2697	-4.74347	0.5439	**C**	-9.98917	-4.70842	-0.1344
C	-10.1901	-4.97196	0.3139	**H**	-8.68337	-5.08027	-1.52023	**H**	-8.74926	-5.59943	-0.69676	**H**	-8.67978	-5.14849	-1.77871

H	-8.82752	-5.45294	-1.26547	**C**	-9.31619	-3.78061	2.09281	**C**	-9.47004	-3.20316	2.22123	**C**	-8.9641	-3.46437	1.67141
C	-9.29393	-3.553	2.06964	**H**	-7.226	-3.29332	2.09869	**H**	-7.38582	-2.87078	2.25625	**H**	-6.92492	-2.98392	1.42217
H	-7.23962	-2.95479	1.82561	**C**	-11.2704	-5.37825	-0.67801	**C**	-11.3221	-5.42161	-0.08102	**C**	-11.1144	-5.32939	-0.6956
C	-11.2511	-5.70211	-0.24233	**C**	-10.4096	-4.33411	1.37214	**C**	-10.5324	-3.87835	1.60086	**C**	-10.0871	-4.09993	1.1178
C	-10.3622	-4.28503	1.52006	**H**	-9.48338	-3.42396	3.10632	**H**	-9.66439	-2.54147	3.03994	**H**	-9.03439	-2.97615	2.62117
H	-9.42734	-3.02581	2.99055	**C**	-12.5242	-5.4533	-0.11377	**C**	-12.5959	-5.23172	0.3448	**C**	-12.2876	-5.35054	-0.01149
C	-12.488	-5.74815	0.41345	**H**	-11.097	-5.74641	-1.68632	**H**	-11.1208	-6.08849	-0.89357	**H**	-11.0492	-5.78801	-1.66003
H	-11.1152	-6.22524	-1.16556	**C**	-11.7144	-4.4272	1.92423	**C**	-11.8546	-3.69419	2.02992	**C**	-11.305	-4.13441	1.80656
C	-11.6019	-4.33257	2.17783	**C**	-12.75	-4.97385	1.19975	**C**	-12.866	-4.35925	1.41224	**C**	-12.3823	-4.75034	1.25297
C	-12.6638	-5.06373	1.62184	**H**	-13.348	-5.88322	-0.67708	**H**	-13.3981	-5.75119	-0.13601	**H**	-13.146	-5.83025	-0.44074
H	-13.2979	-6.30557	-0.01081	**H**	-11.8824	-4.05889	2.93373	**H**	-12.0684	-3.03164	2.84249	**H**	-11.3887	-3.67788	2.77078
H	-11.738	-3.81126	3.10084	**H**	-13.7441	-5.04011	1.6333	**H**	-13.8746	-4.2189	1.74054	**H**	-13.3121	-4.78019	1.78499
H	-13.6088	-5.09841	2.12311	**C**	5.37809	-6.37794	-0.05877	**C**	5.5897	-6.07112	-1.00654	**C**	5.36389	-6.17607	-0.68279
C	5.42015	-6.33141	-0.74817	**C**	6.39445	-6.56494	-0.96439	**C**	6.81837	-6.38734	-1.48296	**C**	6.50903	-6.43042	-1.36459
C	6.47608	-7.08684	-1.27174	**C**	5.6411	-5.94206	1.26452	**C**	5.44874	-5.40259	0.21838	**C**	5.41421	-5.66874	0.62558
C	5.68667	-5.2017	0.03743	**C**	7.74175	-6.32101	-0.58641	**C**	7.95322	-6.08694	-0.72949	**C**	7.75123	-6.21033	-0.76054
C	7.80014	-6.7313	-1.01278	**H**	6.1598	-6.9072	-1.96791	**H**	6.92017	-6.87061	-2.43175	**H**	6.46254	-6.80351	-2.36497
H	6.26354	-7.94566	-1.8729	**C**	6.93736	-5.69283	1.64834	**C**	6.54274	-5.08158	0.95461	**C**	6.61217	-5.44435	1.22908
C	7.02183	-4.83556	0.29246	**H**	4.81575	-5.81879	1.95846	**H**	4.47236	-5.14637	0.57286	**H**	4.50523	-5.45912	1.15151
H	4.88316	-4.62044	0.43893	**C**	8.82365	-6.50214	-1.48933	**C**	9.22194	-6.44137	-1.19475	**C**	8.9405	-6.4871	-1.45123
C	8.84525	-7.50735	-1.53613	**C**	8.02144	-5.8709	0.74567	**C**	7.81911	-5.43273	0.4938	**C**	7.80405	-5.71626	0.54046
C	8.07733	-5.60469	-0.23334	**H**	7.14828	-5.36145	2.66215	**H**	6.42802	-4.56349	1.88446	**H**	6.64651	-5.06284	2.22789
H	7.23544	-3.97238	0.88554	**C**	10.11899	-6.2508	-1.09579	**C**	10.31842	-6.15898	-0.45002	**C**	10.13748	-6.27734	-0.8483
C	10.17504	-7.15133	-1.2793	**H**	8.6108	-6.84288	-2.49968	**H**	9.32584	-6.93723	-2.13746	**H**	8.90393	-6.86547	-2.45233
H	8.62711	-8.37029	-2.12979	**C**	9.36873	-5.62248	1.11924	**C**	8.96222	-5.13782	1.24636	**C**	9.04979	-5.50074	1.1443
C	9.41012	-5.24716	0.0222	**C**	10.39553	-5.80729	0.22063	**C**	10.18783	-5.49912	0.78327	**C**	10.1925	-5.77818	0.46325
C	10.45755	-6.02182	-0.50197	**H**	10.93683	-6.39312	-1.79696	**H**	11.28773	-6.44128	-0.80585	**H**	11.04476	-6.4936	-1.37538
H	10.97374	-7.74284	-1.6779	**H**	9.57644	-5.28258	2.13122	**H**	8.87266	-4.6299	2.1848	**H**	9.10152	-5.11852	2.14168
H	9.62806	-4.38564	0.61543	**H**	11.42235	-5.61359	0.51827	**H**	11.06086	-5.28055	1.36163	**H**	11.14158	-5.6163	0.92797

H	11.47341	-5.74864	-0.30619	**C**	7.84976	4.17405	0.21763	**C**	7.79524	4.22344	0.73485	**C**	7.69529	4.11774	-0.26844
C	7.89074	4.20561	0.11044	**C**	8.87862	4.71917	-0.51438	**C**	8.79599	4.92327	0.14281	**C**	8.78864	4.70008	-0.83037
C	8.95392	4.92791	-0.44413	**C**	8.06001	3.70304	1.5393	**C**	8.08031	3.29093	1.74933	**C**	7.79529	3.4726	0.97363
C	8.09775	3.42045	1.25459	**C**	10.18055	4.81874	0.04327	**C**	10.12001	4.71965	0.52734	**C**	10.00816	4.71072	-0.14385
C	10.21804	4.89726	0.15116	**H**	8.68379	5.07887	-1.52035	**H**	8.56679	5.6342	-0.62375	**H**	8.71673	5.15559	-1.79598
H	8.79482	5.50963	-1.32635	**C**	9.31554	3.78093	2.09349	**C**	9.3671	3.0878	2.14396	**C**	8.97421	3.46392	1.65258
C	9.37014	3.38896	1.85574	**H**	7.2253	3.29389	2.09908	**H**	7.28648	2.74134	2.21373	**H**	6.9371	2.98753	1.39062
H	7.29273	2.85223	1.67324	**C**	11.27063	5.37696	-0.67762	**C**	11.15628	5.42644	-0.09483	**C**	11.13583	5.33071	-0.69941
C	11.26984	5.63662	-0.40946	**C**	10.40916	4.33395	1.37283	**C**	10.40848	3.804	1.53471	**C**	10.0991	4.10167	1.1076
C	10.42927	4.13072	1.30206	**H**	9.48244	3.42476	3.10722	**H**	9.58649	2.38124	2.9174	**H**	9.04127	2.97329	2.60174
H	9.53307	2.80103	2.73418	**C**	12.52428	5.45215	-0.11309	**C**	12.43903	5.22165	0.29105	**C**	12.30438	5.35517	-0.00831
C	12.537	5.61277	0.18691	**H**	11.0975	5.74464	-1.68615	**H**	10.93647	6.1279	-0.87313	**H**	11.07641	5.78629	-1.66507
H	11.10393	6.2201	-1.29058	**C**	11.71387	4.42715	1.92521	**C**	11.73725	3.61104	1.92745	**C**	11.3125	4.13738	1.80442
C	11.6992	4.10842	1.90063	**C**	12.74972	4.97332	1.20072	**C**	12.73236	4.30655	1.31683	**C**	12.392	4.7565	1.25807
C	12.75204	4.84925	1.34036	**H**	13.34834	5.88169	-0.67641	**H**	13.23233	5.75811	-0.18747	**H**	13.16407	5.83575	-0.43249
H	13.33998	6.17749	-0.2407	**H**	11.8816	4.05933	2.93493	**H**	11.96936	2.9158	2.70587	**H**	11.39065	3.67934	2.76713
H	11.86524	3.52682	2.78182	**H**	13.74368	5.03968	1.63449	**H**	13.74775	4.15731	1.62032	**H**	13.31758	4.78969	1.79632
H	13.72015	4.83097	1.79639	**C**	-5.37782	6.37803	-0.06043	**C**	-5.44616	6.12721	-1.02341	**C**	-5.36724	6.16755	-0.67849
C	-5.44836	6.39222	-0.08672	**C**	-6.39507	6.5659	-0.96488	**C**	-6.66666	6.44812	-1.51549	**C**	-6.51103	6.42389	-1.36021
C	-6.28488	7.2325	-0.83247	**C**	-5.63969	5.94207	1.26308	**C**	-5.32481	5.46532	0.21261	**C**	-5.4173	5.66226	0.63187
C	-5.92246	5.1555	0.37015	**C**	-7.74211	6.32282	-0.58547	**C**	-7.81389	6.14419	-0.77972	**C**	-7.75365	6.20786	-0.75587
C	-7.61075	6.86513	-1.08424	**H**	-6.16129	6.9082	-1.96859	**H**	-6.7521	6.93743	-2.46271	**H**	-6.46299	6.79477	-2.36155
H	-5.90841	8.16093	-1.20687	**C**	-6.9357	5.69364	1.64825	**C**	-6.43062	5.15096	0.93218	**C**	-6.61581	5.43908	1.23444
C	-7.25611	4.78749	0.12348	**H**	-4.8137	5.81811	1.95613	**H**	-4.35512	5.20911	0.58868	**H**	-4.50803	5.45387	1.15823
H	-5.27588	4.49789	0.91246	**C**	-8.82489	6.50488	-1.48717	**C**	-9.07925	6.4928	-1.26204	**C**	-8.94261	6.48759	-1.44637
C	-8.44586	7.72096	-1.81803	**C**	-8.02066	5.87263	0.74682	**C**	-7.69667	5.49062	0.44528	**C**	-7.80757	5.71405	0.54589
C	-8.10015	5.64601	-0.60231	**H**	-7.14573	5.36222	2.66223	**H**	-6.33544	4.64459	1.87049	**H**	-6.65002	5.05672	2.23233
H	-7.62945	3.85475	0.48876	**C**	-10.12	6.25434	-1.09225	**C**	-10.1849	6.19093	-0.53688	**C**	-10.1399	6.27883	-0.84358
C	-9.77747	7.3591	-2.06117	**H**	-8.61291	6.84568	-2.49767	**H**	-9.17464	6.99855	-2.19914	**H**	-8.90495	6.8673	-2.44593

H	-8.06759	8.65008	-2.18917	**C**	-9.36769	5.62505	1.12182	**C**	-8.84666	5.1831	1.17854	**C**	-9.05424	5.50205	1.15077
C	-9.43495	5.28589	-0.84291	**C**	-10.3954	5.81075	0.22439	**C**	-10.0673	5.52552	0.69545	**C**	-10.1961	5.78054	0.46835
C	-10.2717	6.14307	-1.57415	**H**	-10.9385	6.39737	-1.79249	**H**	-11.1531	6.46075	-0.90575	**H**	-11.0465	6.49552	-1.37092
H	-10.4155	8.01233	-2.62017	**H**	-9.57452	5.28509	2.13396	**H**	-8.76247	4.6784	2.11844	**H**	-9.1077	5.12225	2.14824
H	-9.81405	4.3585	-0.47048	**H**	-11.422	5.61769	0.52311	**H**	-10.9455	5.28789	1.25672	**H**	-11.1462	5.62007	0.9326
H	-11.289	5.86705	-1.75864	**Ni**	-0.00001	-0.00028	-0.3309	**Ti**	-0.07292	-0.07919	-0.54836	**Mn**	0.02033	0.00781	1.12321
								O	-0.03943	-0.21039	-2.2863	**Cl**	-0.10035	-0.03711	3.28018

Table S6. Optimised cartesian coordinates for MPcs **3c, 4c, 5c** and **6c**.

3c				**4c**				**5c**				**6c**			
C	-3.6169	-2.12223	-0.36319	**C**	3.58712	2.15914	-0.14801	**C**	3.67041	2.1394	-0.04219	**C**	-3.6138	-2.17037	-0.22911
C	-4.11667	-0.88563	-0.28573	**C**	4.09946	0.85134	-0.13703	**C**	4.13764	0.88194	-0.03772	**C**	-4.1132	-0.85917	-0.15504
C	-5.48872	-0.63687	-0.2144	**C**	5.47675	0.62232	-0.14059	**C**	5.50015	0.60881	-0.09464	**C**	-5.48858	-0.61701	-0.17197
C	-6.3538	-1.75729	-0.26348	**C**	6.32748	1.72465	-0.15193	**C**	6.37847	1.74161	-0.14564	**C**	-6.34566	-1.70851	-0.25688
C	-5.80366	-3.06132	-0.39629	**C**	5.80041	3.03358	-0.15092	**C**	5.83248	3.0661	-0.18568	**C**	-5.83178	-3.02339	-0.31941
C	-4.41262	-3.24697	-0.40919	**C**	4.42421	3.27184	-0.15164	**C**	4.44293	3.23902	-0.12406	**C**	-4.4614	-3.27451	-0.3112
C	-2.10441	-1.99878	-0.38814	**C**	2.14297	2.02744	-0.14528	**C**	2.17241	2.06012	-0.03989	**C**	-2.16577	-2.06011	-0.19397
C	-2.9191	0.06394	-0.28504	**C**	2.95573	-0.03144	-0.128	**C**	3.02439	0.01063	-0.02229	**C**	-2.96058	0.02093	-0.08013
H	-7.41382	-1.6225	-0.20575	**H**	7.4032	1.58614	-0.16843	**H**	7.43478	1.59005	-0.16349	**H**	-7.42008	-1.56056	-0.28296
H	-3.98503	-4.22583	-0.46487	**H**	4.04091	4.28602	-0.1579	**H**	4.00029	4.19449	-0.16352	**H**	-4.08549	-4.28979	-0.36745
N	-1.76417	-0.67004	-0.35421	**N**	1.78154	0.69636	-0.13324	**N**	1.85376	0.74499	0.1161	**N**	-1.80064	-0.7302	-0.09847
N	-1.34207	-3.02616	-0.4535	**N**	1.33788	3.09394	-0.15388	**N**	1.33026	3.09181	-0.23717	**N**	-1.36609	-3.11098	-0.23751
N	-3.042	1.32971	-0.22508	**N**	3.08758	-1.36273	-0.1155	**N**	3.11299	-1.32158	-0.19678	**N**	-3.066	1.33824	-0.05436
C	-2.03745	2.11617	-0.19014	**C**	2.0393	-2.14086	-0.10642	**C**	2.06595	-2.06004	-0.43272	**C**	-2.01946	2.14551	-0.0854
C	-2.17299	3.63649	-0.09089	**C**	2.165	-3.60377	-0.0919	**C**	2.16397	-3.62731	-0.28858	**C**	-2.14901	3.59259	-0.16424
C	-0.9197	4.12031	-0.12086	**C**	0.86543	-4.11238	-0.08401	**C**	0.9085	-4.1085	-0.2711	**C**	-0.84348	4.10594	-0.24084
C	-3.29666	4.46359	0.00813	**C**	3.28297	-4.42639	-0.07923	**C**	3.26391	-4.47638	-0.10625	**C**	-3.26956	4.42287	-0.16874
C	0.02536	2.9266	-0.20873	**C**	-0.03446	-2.96015	-0.0975	**C**	-0.04887	-2.88486	-0.40978	**C**	0.05036	2.96932	-0.2039

C	-0.63585	5.47306	-0.08029	**C**	0.63441	-5.48496	-0.06153	**C**	0.62853	-5.4757	-0.08663	**C**	-0.62005	5.48464	-0.32823
C	-3.05047	5.85514	0.05884	**C**	3.0467	-5.80927	-0.06614	**C**	3.02817	-5.88359	-0.01117	**C**	-3.03372	5.79449	-0.2604
H	-4.28871	4.06416	0.04214	**H**	4.28593	-4.01602	-0.07426	**H**	4.24719	-4.06173	0.01796	**H**	-4.27059	4.01438	-0.09673
C	-1.72318	6.35089	0.0053	**C**	1.74224	-6.33253	-0.05526	**C**	1.70915	-6.36797	-0.02892	**C**	-1.72522	6.32249	-0.33902
H	-1.55278	7.40672	0.03437	**H**	1.62468	-7.41115	-0.04061	**H**	1.53772	-7.4178	0.03204	**H**	-1.61533	7.40002	-0.40428
N	-0.70651	1.77665	-0.23412	**N**	0.69862	-1.77674	-0.10968	**N**	0.65743	-1.64659	-0.83414	**N**	-0.68377	1.79869	-0.10694
C	-0.07887	-2.92543	-0.53118	**C**	0.0382	2.9551	-0.1525	**C**	0.07761	2.90093	-0.51695	**C**	-0.04974	-2.99318	-0.1916
C	0.87692	-4.09159	-0.66375	**C**	-0.86165	4.10737	-0.16459	**C**	-0.90581	4.09278	-0.37393	**C**	0.84416	-4.12948	-0.22188
C	2.1341	-3.58324	-0.71779	**C**	-2.16124	3.5988	-0.15873	**C**	-2.16546	3.60825	-0.37624	**C**	2.14922	-3.61662	-0.13761
C	0.60861	-5.44358	-0.72922	**C**	-0.6305	5.47995	-0.18584	**C**	-0.64303	5.45179	-0.18587	**C**	0.6218	-5.50772	-0.32043
C	2.02357	-2.0471	-0.62143	**C**	-2.03558	2.13585	-0.14644	**C**	-2.05342	2.07052	-0.50977	**C**	2.01913	-2.16846	-0.06515
C	3.26168	-4.40757	-0.83868	**C**	-3.27915	4.42151	-0.17217	**C**	-3.28231	4.45644	-0.1932	**C**	3.27032	-4.44519	-0.14467
C	1.70279	-6.30843	-0.8384	**C**	-1.73826	6.3276	-0.19274	**C**	-1.71737	6.34659	-0.16917	**C**	1.72689	-6.34523	-0.3207
C	3.02447	-5.80195	-0.89744	**C**	-3.04275	5.80437	-0.18398	**C**	-3.04226	5.87168	-0.23955	**C**	3.03586	-5.81848	-0.22953
H	4.25317	-4.00347	-0.87954	**H**	-4.28215	4.01124	-0.17925	**H**	-4.2793	4.06956	-0.04357	**H**	4.27198	-4.03579	-0.09031
N	0.71303	-1.69563	-0.51851	**N**	-0.69487	1.77172	-0.14193	**N**	-0.65538	1.62527	-0.92622	**N**	0.6835	-1.82114	-0.09462
N	1.29334	3.04735	-0.24966	**N**	-1.33412	-3.09898	-0.09737	**N**	-1.28601	-3.04062	-0.09442	**N**	1.36718	3.08738	-0.24224
N	3.02813	-1.27014	-0.62335	**N**	-3.08384	1.35769	-0.141	**N**	-3.0818	1.32425	-0.18589	**N**	3.06483	-1.36132	-0.03054
C	2.90671	-0.0032	-0.50346	**C**	-2.95202	0.02636	-0.13049	**C**	-2.99857	-0.00261	0.02105	**C**	2.95942	-0.0436	-0.06251
C	4.10243	0.94431	-0.48981	**C**	-4.09568	-0.85645	-0.12827	**C**	-4.10003	-0.87355	0.00013	**C**	4.11297	0.83529	-0.13538
C	3.59714	2.18022	-0.40098	**C**	-3.58338	-2.16428	-0.11544	**C**	-3.61966	-2.13041	0.02003	**C**	3.61494	2.14654	-0.21785
C	5.47049	0.6932	-0.54826	**C**	-5.4729	-0.62775	-0.1422	**C**	-5.46214	-0.62087	-0.07484	**C**	5.48812	0.59124	-0.14532
C	2.07922	2.04674	-0.33118	**C**	-2.13922	-2.0325	-0.11009	**C**	-2.13441	-2.01288	0.05517	**C**	2.16674	2.03737	-0.18958
C	4.39005	3.30678	-0.38464	**C**	-4.42038	-3.27688	-0.10517	**C**	-4.41753	-3.24754	-0.06171	**C**	4.46418	3.24934	-0.30127
C	6.33172	1.81422	-0.54233	**C**	-6.32371	-1.73013	-0.14028	**C**	-6.33429	-1.74433	-0.13543	**C**	6.34663	1.68146	-0.23146
C	5.77836	3.12306	-0.49243	**C**	-5.79673	-3.03886	-0.11578	**C**	-5.79601	-3.06887	-0.1533	**C**	5.83424	2.99649	-0.3023
H	7.39238	1.67771	-0.58014	**H**	-7.39923	-1.59158	-0.16497	**H**	-7.40159	-1.58585	-0.15916	**H**	7.42097	1.53227	-0.25289
N	1.7457	0.72722	-0.39008	**N**	-1.7778	-0.70142	-0.1206	**N**	-1.84805	-0.72762	0.15395	**N**	1.80042	0.70734	-0.09039
H	3.96372	4.28475	-0.30423	**H**	-4.03707	-4.29101	-0.0935	**H**	-3.97744	-4.21073	-0.07733	**H**	4.08986	4.26484	-0.36414

H	-0.39289	-5.81537	-0.69709	**H**	0.37985	5.87583	-0.19209	**H**	0.36247	5.82038	-0.05933	**H**	-0.38555	-5.90527	-0.38853
H	-5.87125	0.35943	-0.13114	**H**	5.87256	-0.38831	-0.14419	**H**	5.87453	-0.40331	-0.11837	**H**	-5.87533	0.39597	-0.12726
H	0.37057	5.83431	-0.11232	**H**	-0.3759	-5.88091	-0.05427	**H**	-0.3812	-5.85318	0.01343	**H**	0.38787	5.88211	-0.38743
H	5.85227	-0.30494	-0.60229	**H**	-5.86877	0.38262	-0.16442	**H**	-5.80944	0.38428	-0.1206	**H**	5.87334	-0.42206	-0.09532
C	-5.41826	6.40544	-0.12006	**C**	5.31431	-6.46547	-0.5099	**C**	5.32451	-6.5414	-0.46571	**C**	-5.32639	6.43259	-0.60378
C	-6.34261	6.36178	0.93039	**C**	6.40996	-6.77341	0.29384	**C**	6.45625	-6.82431	0.25932	**C**	-6.35301	6.83993	0.24642
C	-5.8219	6.07326	-1.41873	**C**	5.49132	-5.99068	-1.81178	**C**	5.46246	-6.00624	-1.79374	**C**	-5.61329	5.836	-1.83429
C	-7.70661	6.21347	0.64748	**C**	7.70924	-6.60456	-0.20399	**C**	7.72762	-6.59245	-0.24649	**C**	-7.6883	6.65299	-0.13473
H	-6.01022	6.47733	1.94166	**H**	6.22384	-7.14675	1.2948	**H**	6.33739	-7.20626	1.23235	**H**	-6.07555	7.34148	1.16953
C	-7.18258	5.85855	-1.68723	**C**	6.78749	-5.81487	-2.30081	**C**	6.76959	-5.80587	-2.32421	**C**	-6.94546	5.65336	-2.20789
H	-5.09921	5.98847	-2.20249	**H**	4.62691	-5.76896	-2.42956	**H**	4.61308	-5.7398	-2.40496	**H**	-4.80346	5.53278	-2.48979
C	-8.1308	6.00456	-0.66477	**C**	7.89025	-6.11828	-1.50734	**C**	7.89014	-6.1303	-1.54867	**C**	-7.98092	6.06568	-1.37188
H	-7.49821	5.58496	-2.67136	**H**	6.93009	-5.44654	-3.31279	**H**	6.91518	-5.42	-3.31634	**H**	-7.17262	5.19651	-3.16671
O	-4.08254	6.83212	0.16338	**O**	4.05819	-6.74004	0.00551	**O**	4.08651	-6.83392	0.16332	**O**	-4.03569	6.73984	-0.21718
C	-7.86373	-4.2288	0.15628	**C**	7.82491	4.19627	0.42607	**C**	7.81104	4.27803	0.41921	**C**	-7.86474	-4.19417	0.19387
C	-8.02409	-3.7927	1.4835	**C**	7.99697	3.71154	1.72541	**C**	7.97228	3.72719	1.71618	**C**	-8.01023	-3.79674	1.52682
C	-8.95043	-4.72911	-0.54355	**C**	8.86897	4.84046	-0.23716	**C**	8.89215	4.89246	-0.20126	**C**	-8.92658	-4.77331	-0.49796
C	-9.27446	-3.96007	2.11752	**C**	9.23593	3.86765	2.35123	**C**	9.22024	3.85425	2.37067	**C**	-9.24063	-3.973	2.16221
H	-7.20751	-3.34657	2.01221	**H**	7.17275	3.22513	2.23683	**H**	7.17059	3.20199	2.20207	**H**	-7.16963	-3.3616	2.05759
C	-10.1733	-4.91982	0.07955	**C**	10.10673	5.00366	0.39841	**C**	10.12588	4.98858	0.4311	**C**	-10.1526	-4.95397	0.15313
H	-8.83759	-4.98604	-1.57515	**H**	8.68736	5.20643	-1.24172	**H**	8.77497	5.27931	-1.18359	**H**	-8.78808	-5.08049	-1.52758
C	-10.3446	-4.5551	1.42079	**C**	10.28555	4.50703	1.69846	**C**	10.27642	4.51167	1.73339	**C**	-10.3123	-4.54896	1.48458
H	-9.41112	-3.63734	3.12935	**H**	9.37251	3.49177	3.36141	**H**	9.36317	3.46218	3.3595	**H**	-9.35503	-3.66501	3.19747
O	-6.61781	-4.21789	-0.5425	**O**	6.61151	4.14709	-0.23403	**O**	6.59073	4.26846	-0.31079	**O**	-6.65783	-4.11634	-0.47635
C	7.86964	4.2181	0.06198	**C**	-7.83255	-4.18716	0.45098	**C**	-7.82054	-4.259	0.44021	**C**	7.86513	4.16821	0.21617
C	8.08319	3.66365	1.33656	**C**	-8.02516	-3.68571	1.74105	**C**	-8.0021	-3.69553	1.72573	**C**	8.00171	3.77872	1.55242
C	8.93205	4.76237	-0.64253	**C**	-8.86861	-4.83182	-0.22404	**C**	-8.89226	-4.88277	-0.19088	**C**	8.93213	4.74175	-0.47242
C	9.36168	3.76361	1.92618	**C**	-9.27656	-3.82558	2.3455	**C**	-9.26124	-3.8108	2.36231	**C**	9.22825	3.95739	2.19454
H	7.28532	3.17877	1.85982	**H**	-7.2069	-3.19898	2.2617	**H**	-7.20364	-3.17411	2.22569	**H**	7.1572	3.34775	2.08037

C	10.18462	4.88371	-0.06067	**C**	-10.1192	-4.97868	0.39021	**C**	-10.1273	-4.98354	0.43294	**C**	10.15423	4.92479	0.18531
H	8.7775	5.10794	-1.64241	**H**	-8.67108	-5.21113	-1.22061	**H**	-8.7688	-5.25871	-1.17661	**H**	8.8006	5.04262	-1.50481
C	10.40727	4.4082	1.23724	**C**	-10.3185	-4.46538	1.68075	**C**	-10.3086	-4.47416	1.71795	**C**	10.30493	4.52782	1.52023
H	9.53853	3.3517	2.8986	**H**	-9.42924	-3.43681	3.34847	**H**	-9.42207	-3.39936	3.34128	**H**	9.33563	3.65568	3.2324
O	6.59073	4.28593	-0.57035	**O**	-6.60605	-4.15439	-0.18568	**O**	-6.5811	-4.2524	-0.25781	**O**	6.66241	4.08777	-0.461
O	4.05864	-6.77537	-1.0143	**O**	-4.05413	6.73521	-0.2564	**O**	-4.06276	6.87548	-0.32597	**O**	4.0396	-6.75604	-0.28788
C	5.39731	-6.35229	-0.74326	**C**	-5.31116	6.45942	0.25613	**C**	-5.3243	6.53922	0.28754	**C**	5.30253	-6.47583	0.20901
C	5.81968	-6.03134	0.55253	**C**	-5.4903	5.98818	1.559	**C**	-5.48198	5.99761	1.56896	**C**	5.49176	-6.07813	1.53592
C	6.30592	-6.30191	-1.8059	**C**	-6.40548	6.76235	-0.5513	**C**	-6.45065	6.8135	-0.50003	**C**	6.3869	-6.70003	-0.63399
C	7.18464	-5.81979	0.80268	**C**	-6.78725	5.81115	2.04547	**C**	-6.77744	5.79747	2.06899	**C**	6.78931	-5.89453	2.01529
H	5.10863	-5.95301	1.3476	**H**	-4.6268	5.77035	2.17946	**H**	-4.62189	5.73797	2.14697	**H**	4.63207	-5.92155	2.17982
C	7.67337	-6.15608	-1.54282	**C**	-7.7056	6.59218	-0.0561	**C**	-7.72423	6.57926	-0.02352	**C**	7.6856	-6.52168	-0.13974
H	5.95847	-6.41043	-2.81281	**H**	-6.21773	7.13293	-1.55298	**H**	-6.3231	7.18901	-1.50118	**H**	6.21493	-7.01598	-1.65588
C	8.11756	-5.95701	-0.23543	**C**	-7.88872	6.10972	1.24836	**C**	-7.88948	6.11747	1.28421	**C**	7.88634	-6.11475	1.18505
H	7.51516	-5.55547	1.7845	**H**	-6.93158	5.44582	3.05831	**H**	-6.9146	5.41975	3.05993	**H**	6.94056	-5.58692	3.0458
H	1.54053	-7.36477	-0.88054	**H**	-1.62064	7.40622	-0.20663	**H**	-1.53258	7.41051	-0.07957	**H**	1.61781	-7.42265	-0.38929
Co	-0.0061	0.02985	-0.37216	**H**	11.25188	4.638	2.17285	**H**	11.21042	4.6362	2.23402	**H**	-11.2731	-4.69577	1.96519
H	-11.2835	-4.71916	1.90836	**H**	8.9031	-5.99156	-1.87375	**H**	8.87192	-5.99973	-1.93993	**H**	-9.01998	5.94562	-1.65781
H	-9.17539	5.93551	-0.8831	**H**	-11.2944	-4.58396	2.13852	**H**	-11.2603	-4.56043	2.18943	**H**	11.26291	4.6764	2.00601
H	11.3672	4.52477	1.6965	**H**	-8.9022	5.98206	1.61268	**H**	-8.87033	5.99249	1.68033	**H**	8.90148	-5.98166	1.54254
H	9.16531	-5.88913	-0.03237	**C**	11.26579	5.69075	-0.26591	**C**	11.30195	5.6371	-0.30827	**C**	-11.3214	-5.56759	-0.53435
C	-11.2928	-5.548	-0.75821	**O**	12.3349	5.79967	0.3138	**O**	12.44931	5.62276	0.2119	**O**	-12.4101	-5.74531	-0.02663
O	-12.2547	-6.14576	-0.21144	**C**	-8.92537	6.90386	-0.87663	**C**	-8.94273	6.83678	-0.92061	**C**	8.88652	-6.74834	-0.9894
C	8.68194	-6.22632	-2.69765	**O**	-10.0416	6.72798	-0.41445	**O**	-10.0899	6.52427	-0.51641	**O**	10.03415	-6.60048	-0.62101
O	9.7448	-6.89165	-2.57669	**C**	-11.2707	-5.66528	-0.28759	**C**	-11.3051	-5.63213	-0.31987	**C**	11.32826	5.53246	-0.49849
C	11.28089	5.56025	-0.89108	**O**	-12.351	-5.7604	0.27363	**O**	-12.4498	-5.63352	0.1921	**O**	12.41433	5.71093	0.01475
O	12.25429	6.13189	-0.33661	**C**	8.93022	-6.92167	0.61257	**C**	8.94731	-6.85646	0.65395	**C**	-8.84298	7.08396	0.7235
C	-8.73499	6.29107	1.78437	**O**	10.0458	-6.74622	0.14863	**O**	10.09444	-6.54277	0.25201	**O**	-9.95037	7.28722	0.28689
O	-9.78871	6.9675	1.64567	**C**	11.0847	6.24824	-1.66781	**C**	11.0928	6.26886	-1.70389	**H**	-7.54374	7.36393	2.20641

C	-11.2063	-5.42496	-2.29224	**C**	-11.068	-6.23954	-1.67972	**C**	-11.0847	-6.25603	-1.71796	**H**	9.36016	-7.76903	-2.62912
C	11.15854	5.51734	-2.42652	**C**	-8.74493	7.4407	-2.28627	**C**	-8.75205	7.45058	-2.32647	**H**	11.972	5.80785	-2.36016
C	8.38828	-5.45988	-3.99386	**C**	8.75194	-7.46363	2.02056	**C**	8.75871	-7.47416	2.06056	**H**	-11.9535	-5.85454	-2.3983
C	-8.47367	5.51846	3.08361	**H**	10.28205	6.99489	-1.69487	**H**	10.15152	6.79129	-1.73191	**Mn**	-0.00063	-0.01128	0.21472
H	-10.5526	-6.17342	-2.68389	**H**	12.02092	6.71215	-1.98237	**H**	11.89715	6.95414	-1.92392	**Cl**	-0.0077	-0.00357	2.398
H	-12.1814	-5.5453	-2.71426	**H**	10.817	5.45551	-2.37667	**H**	11.08206	5.47324	-2.43363	**C**	8.5774	-7.14599	-2.24962
H	-10.8265	-4.45317	-2.5429	**H**	8.18537	-8.40248	2.01327	**H**	7.99876	-8.24146	2.02269	**C**	-11.0571	-5.92214	-1.81784
H	-7.78723	6.04403	3.70451	**H**	9.73763	-7.6396	2.45422	**H**	9.68965	-7.91263	2.39495	**C**	-8.59547	7.24222	2.05162
H	-9.40008	5.3861	3.60428	**H**	8.20065	-6.75449	2.64974	**H**	8.45737	-6.69842	2.738	**C**	11.07238	5.88049	-1.78543
H	-8.06668	4.55783	2.83003	**H**	-10.7806	-5.45687	-2.39204	**H**	-10.9771	-5.45818	-2.42843	**H**	10.33449	5.22156	-2.19314
H	11.77251	4.7213	-2.8001	**H**	-10.271	-6.99275	-1.68351	**H**	-10.1709	-6.87365	-1.70485	**H**	10.70898	6.88638	-1.81737
H	10.13889	5.3378	-2.70007	**H**	-12.0018	-6.69958	-2.00672	**H**	-11.9054	-6.86539	-1.9842	**H**	7.65944	-7.69557	-2.23513
H	11.4821	6.44374	-2.84573	**H**	-9.72995	7.61283	-2.72296	**H**	-9.68268	7.88671	-2.66426	**H**	8.46889	-6.2869	-2.87818
H	9.30355	-5.31723	-4.53112	**H**	-8.18043	8.38082	-2.28128	**H**	-7.99337	8.22034	-2.28933	**H**	-10.3182	-5.26391	-2.22478
H	7.69764	-5.9958	-4.60138	**H**	-8.19059	6.73032	-2.91134	**H**	-8.4471	6.6736	-2.99985	**H**	-10.6915	-6.92743	-1.8421
H	7.97361	-4.50388	-3.73555	**Ni**	0.00187	-0.00252	-0.1259	**Ti**	0.00195	0.00838	0.13498	**H**	-9.1113	8.10855	2.40981
								O	-0.25462	0.61366	1.72356	**H**	-8.93667	6.37868	2.58339

Table S7. Optimised cartesian coordinates for MPcs **3d, 4d, 5d** and **6d**.

3d				**4d**				**5d**				**6d**			
C	3.58712	2.15914	-0.14801	**C**	-3.57237	-2.16799	-0.18909	**C**	-3.64331	-2.13815	0.04349	**C**	-3.61676	2.22265	-0.1041
C	4.09946	0.85134	-0.13703	**C**	-4.08319	-0.86232	-0.16975	**C**	-4.14476	-0.82191	0.0245	**C**	-4.13842	0.91438	-0.12838
C	5.47675	0.62232	-0.14059	**C**	-5.46035	-0.63155	-0.14593	**C**	-5.51395	-0.58234	-0.11211	**C**	-5.51305	0.6933	-0.01895
C	6.32748	1.72465	-0.15193	**C**	-6.30907	-1.73331	-0.13961	**C**	-6.3667	-1.67569	-0.21613	**C**	-6.35043	1.79693	0.10116
C	5.80041	3.03358	-0.15092	**C**	-5.78239	-3.04366	-0.14785	**C**	-5.85343	-2.99097	-0.18333	**C**	-5.81661	3.10434	0.11134
C	4.42421	3.27184	-0.15164	**C**	-4.40893	-3.28206	-0.17463	**C**	-4.48702	-3.24154	-0.06062	**C**	-4.44446	3.33615	0.01666
C	2.14297	2.02744	-0.14528	**C**	-2.12304	-2.03854	-0.21451	**C**	-2.19471	-2.02961	0.1745	**C**	-2.16802	2.09501	-0.21567
C	2.95573	-0.03144	-0.128	**C**	-2.93662	0.02759	-0.18502	**C**	-2.99893	0.06473	0.14398	**C**	-3.0044	0.0135	-0.25427

H	7.4032	1.58614	-0.16843	**H**	-7.38514	-1.59586	-0.1361	**H**	-7.43526	-1.5277	-0.32985	**H**	-7.42266	1.66269	0.19576
H	4.04091	4.28602	-0.1579	**H**	-4.02497	-4.29585	-0.18786	**H**	-4.11238	-4.25884	-0.04799	**H**	-4.05406	4.34735	0.0376
N	1.78154	0.69636	-0.13324	**N**	-1.76667	-0.70512	-0.21221	**N**	-1.85408	-0.69672	0.25029	**N**	-1.84623	0.75996	-0.32259
N	1.33788	3.09394	-0.15388	**N**	-1.32192	-3.08687	-0.23458	**N**	-1.37988	-3.07593	0.16952	**N**	-1.33805	3.12863	-0.1694
N	3.08758	-1.36273	-0.1155	**N**	-3.06131	1.34263	-0.17295	**N**	-3.08733	1.38881	0.10532	**N**	-3.11248	-1.30937	-0.2526
C	2.0393	-2.14086	-0.10642	**C**	-2.01201	2.14372	-0.18832	**C**	-2.04055	2.20316	0.1227	**C**	-2.07716	-2.13866	-0.27729
C	2.165	-3.60377	-0.0919	**C**	-2.14216	3.59347	-0.17601	**C**	-2.14653	3.65009	-0.02742	**C**	-2.20617	-3.5868	-0.16699
C	0.86543	-4.11238	-0.08401	**C**	-0.83782	4.10473	-0.19996	**C**	-0.83141	4.15107	-0.02527	**C**	-0.89826	-4.1083	-0.16607
C	3.28297	-4.42639	-0.07923	**C**	-3.26258	4.42309	-0.13957	**C**	-3.25478	4.48442	-0.16932	**C**	-3.32657	-4.41008	-0.06216
C	-0.03446	-2.96015	-0.0975	**C**	0.0524	2.95917	-0.22746	**C**	0.05281	3.00788	0.12561	**C**	0.00464	-2.97428	-0.2742
C	0.63441	-5.48496	-0.06153	**C**	-0.60967	5.48349	-0.18912	**C**	-0.59234	5.52108	-0.16875	**C**	-0.67937	-5.48431	-0.05776
C	3.0467	-5.80927	-0.06614	**C**	-3.02461	5.7982	-0.13796	**C**	-3.00212	5.84979	-0.31089	**C**	-3.09312	-5.78103	0.04871
H	4.28593	-4.01602	-0.07426	**H**	-4.26542	4.01381	-0.10831	**H**	-4.26149	4.08413	-0.16337	**H**	-4.32894	-3.99796	-0.07209
C	1.74224	-6.33253	-0.05526	**C**	-1.71447	6.32425	-0.16089	**C**	-1.68628	6.36355	-0.30962	**C**	-1.78728	-6.31522	0.04883
H	1.62468	-7.41115	-0.04061	**H**	-1.60073	7.40341	-0.15352	**H**	-1.56018	7.43553	-0.42159	**H**	-1.67756	-7.39142	0.13365
N	0.69862	-1.77674	-0.10968	**N**	-0.68006	1.78738	-0.21894	**N**	-0.70976	1.86278	0.22845	**N**	-0.74033	-1.81654	-0.3561
C	0.0382	2.9551	-0.1525	**C**	-0.00682	-2.96169	-0.2578	**C**	-0.05562	-2.98647	0.19678	**C**	-0.01521	3.0201	-0.17909
C	-0.86165	4.10737	-0.16459	**C**	0.88275	-4.10799	-0.28037	**C**	0.83047	-4.13305	0.08741	**C**	0.88586	4.14969	-0.02253
C	-2.16124	3.5988	-0.15873	**C**	2.18802	-3.59647	-0.29941	**C**	2.14587	-3.63196	0.09406	**C**	2.19359	3.62923	-0.02456
C	-0.6305	5.47995	-0.18584	**C**	0.6523	-5.48607	-0.29089	**C**	0.59239	-5.50511	-0.03424	**C**	0.66594	5.52071	0.13764
C	-2.03558	2.13585	-0.14644	**C**	2.05877	-2.14764	-0.29118	**C**	2.03783	-2.18166	0.2043	**C**	2.06601	2.18421	-0.17867
C	-3.27915	4.42151	-0.17217	**C**	3.30663	-4.42884	-0.32995	**C**	3.25495	-4.46948	-0.0179	**C**	3.31295	4.44575	0.12871
C	-1.73826	6.3276	-0.19274	**C**	1.75675	-6.32898	-0.3113	**C**	1.68827	-6.3518	-0.13111	**C**	1.77268	6.3475	0.27615
C	-3.04275	5.80437	-0.18398	**C**	3.06512	-5.80232	-0.32816	**C**	3.00384	-5.83864	-0.12018	**C**	3.08047	5.81517	0.26832
H	-4.28215	4.01124	-0.17925	**H**	4.3115	-4.02342	-0.35876	**H**	4.26171	-4.06894	-0.02659	**H**	4.31344	4.02989	0.14148
N	-0.69487	1.77172	-0.14193	**N**	0.72595	-1.79167	-0.26514	**N**	0.70575	-1.8391	0.28123	**N**	0.7303	1.86417	-0.28587
N	-1.33412	-3.09898	-0.09737	**N**	1.36645	3.08374	-0.25456	**N**	1.37743	3.09685	0.11659	**N**	1.32744	-3.0838	-0.24873
N	-3.08384	1.35769	-0.141	**N**	3.10785	-1.34621	-0.30746	**N**	3.08504	-1.36773	0.18428	**N**	3.10037	1.35464	-0.16571
C	-2.95202	0.02636	-0.13049	**C**	2.98299	-0.03158	-0.3012	**C**	2.99628	-0.0432	0.19061	**C**	2.99231	0.03186	-0.21012

C	-4.09568	-0.85645	-0.12827	**C**	4.12891	0.85933	-0.32279	**C**	4.14399	0.84078	0.06901	**C**	4.12501	-0.87174	-0.09389
C	-3.58338	-2.16428	-0.11544	**C**	3.61593	2.1642	-0.30772	**C**	3.64244	2.15695	0.04971	**C**	3.60468	-2.18054	-0.11979
C	-5.4729	-0.62775	-0.1422	**C**	5.50656	0.62855	-0.35854	**C**	5.51513	0.59844	-0.04019	**C**	5.49712	-0.65252	0.04695
C	-2.13922	-2.0325	-0.11009	**C**	2.16776	2.03406	-0.27675	**C**	2.19185	2.05113	0.15989	**C**	2.15789	-2.05023	-0.25073
C	-4.42038	-3.27688	-0.10517	**C**	4.4528	3.27981	-0.31626	**C**	4.48783	3.25785	-0.06597	**C**	4.432	-3.29644	-0.01972
C	-6.32371	-1.73013	-0.14028	**C**	6.35319	1.7314	-0.37632	**C**	6.36963	1.68934	-0.15528	**C**	6.33385	-1.75855	0.14705
C	-5.79673	-3.03886	-0.11578	**C**	5.82363	3.03987	-0.34889	**C**	5.85605	3.00486	-0.1607	**C**	5.80184	-3.06612	0.10638
H	-7.39923	-1.59158	-0.16497	**H**	7.42933	1.59863	-0.41969	**H**	7.43985	1.53905	-0.24861	**H**	7.40395	-1.62629	0.26558
N	-1.7778	-0.70142	-0.1206	**N**	1.81261	0.70153	-0.27424	**N**	1.84994	0.72026	0.26122	**N**	1.83653	-0.71178	-0.32059
H	-4.03707	-4.29101	-0.0935	**H**	4.06724	4.29303	-0.30425	**H**	4.11319	4.27509	-0.08264	**H**	4.04311	-4.30829	-0.03732
H	0.37985	5.87583	-0.19209	**H**	-0.35781	-5.88236	-0.27865	**H**	-0.42047	-5.89445	-0.04536	**H**	-0.34112	5.92481	0.14642
H	5.87256	-0.38831	-0.14419	**H**	-5.8553	0.37932	-0.1426	**H**	-5.89937	0.43177	-0.1423	**H**	-5.91474	-0.31491	-0.02121
H	-0.3759	-5.88091	-0.05427	**H**	0.3996	5.88181	-0.2066	**H**	0.42027	5.91121	-0.17114	**H**	0.32779	-5.88814	-0.0539
H	-5.86877	0.38262	-0.16442	**H**	5.90147	-0.38198	-0.38317	**H**	5.90079	-0.41602	-0.04152	**H**	5.89689	0.35574	0.0846
C	5.31431	-6.46547	-0.5099	**C**	-5.30709	6.45782	-0.49457	**C**	-5.27684	6.44748	-0.79438	**C**	-5.32138	-6.42638	0.68516
C	6.40996	-6.77341	0.29384	**C**	-6.35966	6.76598	0.36308	**C**	-6.32196	6.81084	0.05147	**C**	-6.45928	-6.91691	0.04524
C	5.49132	-5.99068	-1.81178	**C**	-5.54976	5.97569	-1.78464	**C**	-5.52831	5.83609	-2.02468	**C**	-5.42406	-5.76762	1.91337
C	7.70924	-6.60456	-0.20399	**C**	-7.67732	6.58734	-0.07725	**C**	-7.64717	6.55919	-0.33084	**C**	-7.71816	-6.7507	0.6366
H	6.22384	-7.14675	1.2948	**H**	-6.14721	7.14573	1.35519	**H**	-6.07886	7.29112	0.99286	**H**	-6.31978	-7.46394	-0.88317
C	6.78749	-5.81487	-2.30081	**C**	-6.8662	5.79231	-2.20969	**C**	-6.84884	5.57856	-2.39854	**C**	-6.68185	-5.60609	2.49644
H	4.62691	-5.76896	-2.42956	**H**	-4.71601	5.75381	-2.44315	**H**	-4.70032	5.57301	-2.67542	**H**	-4.5311	-5.39938	2.40726
C	7.89025	-6.11828	-1.50734	**C**	-7.9308	6.09571	-1.36381	**C**	-7.9023	5.93579	-1.56121	**C**	-7.82493	-6.09985	1.8721
H	6.93009	-5.44654	-3.31279	**H**	-7.05769	5.41925	-3.21158	**H**	-7.05053	5.10419	-3.35479	**H**	-6.76342	-5.09999	3.45401
O	4.05819	-6.74004	0.00551	**O**	-4.0268	6.73934	-0.0509	**O**	-3.99213	6.80023	-0.41108	**O**	-4.10863	-6.7143	0.09146
C	7.82491	4.19627	0.42607	**C**	-7.79206	-4.20185	0.47952	**C**	-7.93444	-4.13094	0.19473	**C**	-7.87761	4.2817	-0.25737
C	7.99697	3.71154	1.72541	**C**	-7.91668	-3.73231	1.7911	**C**	-8.2077	-3.67639	1.48737	**C**	-8.14213	3.87257	-1.56823
C	8.86897	4.84046	-0.23716	**C**	-8.86214	-4.82574	-0.15885	**C**	-8.92968	-4.73198	-0.57469	**C**	-8.87347	4.86437	0.52327
C	9.23593	3.86765	2.35123	**C**	-9.13352	-3.88203	2.45846	**C**	-9.49937	-3.81869	1.99954	**C**	-9.4253	4.04078	-2.09123
H	7.17275	3.22513	2.23683	**H**	-7.07009	-3.26153	2.28026	**H**	-7.42044	-3.22408	2.08176	**H**	-7.35136	3.43446	-2.16866

C	10.10673	5.00366	0.39841	**C**	-10.0745	-4.97882	0.52411	**C**	-10.2212	-4.88207	-0.05262	**C**	-10.154	5.03702	-0.01571
H	8.68736	5.20643	-1.24172	**H**	-8.74037	-5.18803	-1.17253	**H**	-8.67064	-5.07639	-1.56969	**H**	-8.64349	5.18128	1.53335
C	10.28555	4.50703	1.69846	**C**	-10.2129	-4.502	1.83397	**C**	-10.5015	-4.41604	1.24074	**C**	-10.4325	4.62077	-1.32386
H	9.37251	3.49177	3.36141	**H**	-9.2315	-3.518	3.47712	**H**	-9.71485	-3.46619	3.0043	**H**	-9.6321	3.72398	-3.10933
O	6.61151	4.14709	-0.23403	**O**	-6.59866	-4.15399	-0.21568	**O**	-6.66485	-4.09219	-0.35418	**O**	-6.61232	4.21375	0.29739
C	-7.83255	-4.18716	0.45098	**C**	7.76942	4.26379	0.34715	**C**	7.93109	4.15386	0.22387	**C**	7.8692	-4.22979	-0.26759
C	-8.02516	-3.68571	1.74105	**C**	7.85069	3.7445	1.64228	**C**	8.18497	3.72783	1.53011	**C**	8.15101	-3.78022	-1.5615
C	-8.86861	-4.83182	-0.22404	**C**	8.82631	5.00399	-0.18612	**C**	8.93753	4.73902	-0.54322	**C**	8.85524	-4.83504	0.50835
C	-9.27656	-3.82558	2.3455	**C**	9.01197	3.95347	2.38891	**C**	9.46866	3.88244	2.05857	**C**	9.44142	-3.93085	-2.07182
H	-7.2069	-3.19898	2.2617	**H**	7.0189	3.1847	2.05613	**H**	7.38897	3.28801	2.12224	**H**	7.36791	-3.32447	-2.15883
C	-10.1192	-4.97868	0.39021	**C**	9.97876	5.2249	0.57706	**C**	10.22083	4.90167	-0.00502	**C**	10.14333	-4.98948	-0.01807
H	-8.67108	-5.21113	-1.22061	**H**	8.73006	5.35541	-1.20973	**H**	8.6934	5.06141	-1.54931	**H**	8.61198	-5.18289	1.50505
C	-10.3185	-4.46538	1.68075	**C**	10.0772	4.68036	1.86406	**C**	10.48182	4.46409	1.30225	**C**	10.43901	-4.53291	-1.3089
H	-9.42924	-3.43681	3.34847	**H**	9.07761	3.54593	3.39367	**H**	9.66905	3.55213	3.07395	**H**	9.6616	-3.58273	-3.0768
O	-6.60605	-4.15439	-0.18568	**O**	6.65056	4.14582	-0.44825	**O**	6.67008	4.10223	-0.34334	**O**	6.59643	-4.17983	0.27154
O	-4.05413	6.73521	-0.2564	**O**	4.07817	-6.7383	-0.42057	**O**	3.99525	-6.78018	-0.27825	**O**	4.08364	6.7354	0.46833
C	-5.31116	6.45942	0.25613	**C**	5.29956	-6.52549	0.18421	**C**	5.28739	-6.5303	0.15573	**C**	5.3742	6.4844	0.03235
C	-5.4903	5.98818	1.559	**C**	5.42338	-6.0062	1.47602	**C**	5.55959	-6.15102	1.47234	**C**	5.64519	6.14111	-1.29571
C	-6.40548	6.76235	-0.5513	**C**	6.42777	-6.93425	-0.52701	**C**	6.32021	-6.76556	-0.74888	**C**	6.40578	6.68098	0.94599
C	-6.78725	5.81115	2.04547	**C**	6.69348	-5.87744	2.04017	**C**	6.8879	-5.99679	1.87438	**C**	6.9702	5.98338	-1.70394
H	-4.6268	5.77035	2.17946	**H**	4.53754	-5.70601	2.02571	**H**	4.74262	-5.98499	2.16733	**H**	4.82684	6.00514	-1.99557
C	-7.7056	6.59218	-0.0561	**C**	7.69724	-6.81924	0.0537	**C**	7.65285	-6.6192	-0.33904	**C**	7.73267	6.52953	0.52302
H	-6.21773	7.13293	-1.55298	**H**	6.28291	-7.29935	-1.54003	**H**	6.06102	-7.06615	-1.75802	**H**	6.17118	6.95446	1.96767
C	-7.88872	6.10972	1.24836	**C**	7.82892	-6.27099	1.3356	**C**	7.92897	-6.22817	0.97943	**C**	8.01474	6.17607	-0.80234
H	-6.93158	5.44582	3.05831	**H**	6.79197	-5.47057	3.04245	**H**	7.10487	-5.7027	2.89738	**H**	7.18418	5.71773	-2.73503
H	-1.62064	7.40622	-0.20663	**H**	1.64135	-7.40796	-0.31753	**H**	1.56327	-7.42617	-0.21879	**H**	1.66214	7.4204	0.39527
Co	0.00187	-0.00252	-0.1259	**H**	-11.1636	-4.62846	2.33999	**H**	-11.5078	-4.53743	1.62615	**H**	-11.4332	4.76274	-1.71672
H	11.25188	4.638	2.17285	**H**	-8.95969	5.9635	-1.67982	**H**	-8.93375	5.7471	-1.83838	**H**	-8.80569	-5.99532	2.32253
H	8.9031	-5.99156	-1.87375	**H**	10.98749	4.84108	2.43071	**H**	11.48214	4.59475	1.70006	**H**	11.44515	-4.66159	-1.69219

H	-11.2944	-4.58396	2.13852	**H**	8.82186	-6.16767	1.75887	**H**	8.96595	-6.11723	1.277	**H**	9.05016	6.06234	-1.10391
H	-8.9022	5.98206	1.61268	**C**	-11.251	-5.63705	-0.10649	**C**	-11.3325	-5.524	-0.834	**C**	-11.2572	5.65488	0.76963
C	11.26579	5.69075	-0.26591	**O**	-12.3293	-5.79251	0.4302	**O**	-12.4486	-5.62718	-0.35007	**O**	-12.3873	5.82805	0.36022
O	12.3349	5.79967	0.3138	**C**	8.95078	-7.22855	-0.66429	**C**	8.81011	-6.86091	-1.26652	**C**	8.87925	6.7284	1.45102
C	-8.92537	6.90386	-0.87663	**O**	10.04205	-6.78688	-0.39524	**O**	9.95663	-6.70551	-0.87676	**O**	10.04786	6.6005	1.14657
O	-10.0416	6.72798	-0.41445	**C**	11.15236	6.00296	0.0557	**C**	11.34352	5.5275	-0.78324	**C**	11.23682	-5.6296	0.76296
C	-11.2707	-5.66528	-0.28759	**O**	12.27231	5.8841	0.49163	**O**	12.45226	5.64162	-0.28502	**O**	12.37286	-5.788	0.36417
O	-12.351	-5.7604	0.27363	**C**	-8.84408	6.90147	0.79168	**C**	-8.81832	6.92867	0.53541	**C**	-8.98041	-7.26917	0.00954
C	8.93022	-6.92167	0.61257	**O**	-10.0065	6.75574	0.47152	**O**	-9.9567	6.67436	0.17506	**O**	-9.99051	-7.48163	0.63636
O	10.0458	-6.74622	0.14863	**O**	8.81279	-8.14418	-1.66119	**H**	-7.94501	6.9976	2.52081	**H**	-8.13667	-7.13682	-1.71658
O	-8.75552	7.40919	-2.20354	**O**	10.90524	6.87754	-0.95715	**H**	9.47905	-7.42945	-3.21311	**H**	9.31691	7.17802	3.21644
O	-11.0799	-6.20572	-1.59771	**O**	-8.48516	7.37928	2.01035	**Ti**	-0.00692	0.01952	0.92117	**O**	10.84213	-6.03316	1.99746
O	8.76241	-7.43181	1.9379	**O**	-11.0073	-6.0616	-1.37262	**O**	-0.01797	0.03663	2.53221	**H**	11.63067	-6.43279	2.40892
O	11.09537	6.2154	-1.58522	**H**	7.91684	-8.51833	-1.64908	**O**	11.09066	5.98689	-2.11363	**O**	-8.95094	-7.49875	-1.33113
H	-7.81882	7.48401	-2.40001	**H**	9.948	6.97624	-1.0865	**H**	11.84743	6.48597	-2.42958	**O**	8.49306	7.07497	2.7051
H	-10.1402	-6.2806	-1.77924	**H**	-11.8379	-6.47106	-1.67783	**O**	-8.56029	7.62227	1.86206	**O**	-10.879	6.0189	2.02149
H	11.95588	6.37266	-1.98069	**H**	-9.32043	7.54868	2.4841	**O**	8.52839	-7.30118	-2.69309	**H**	-11.6725	6.40728	2.43425
H	9.6237	-7.58412	2.3336	**Ni**	0.02291	-0.00199	-0.2429	**O**	-11.0603	-6.01161	-2.15045	**Mn**	0.00006	0.03522	-0.98711
								H	-11.8127	-6.51685	-2.467	**Cl**	0.01472	0.07065	-3.14676

(g) TGA – Tabulated degradation profiles and curves

Table S8. TGA of MPc complexes **(3a-3d, 4a-4d, 5a-5d** and **6a-6d)**.

Metal	Subs.	Weight loss			
		Stage I	**Stage II**	**Stage III**	**Major decomposition temperature (°C)**
Co	**a**	10% (50 °C - 400°C)	75% (400 °C - 800°C)	92% (800 °C - 900°C)	400
	b	10% (50 °C - 400°C)	80% (400 °C - 637°C)	79% (637 °C - 900°C)	400
	c	10% (50 °C - 400°C)	85% (400 °C - 800°C)	92% (800 °C - 900°C)	400
	d	10% (50 °C - 400°C)	68% (400 °C - 670°C)	98% (525 °C - 900°C)	325
Ni	**a**	8% (50 °C - 365°C)	80% (365 °C - 680°C)	80% (680 °C - 900°C)	365
	b	3% (50 °C - 335°C)	79% (335 °C - 635°C)	80% (635 °C - 900°C)	335
	c	7% (50 °C - 350°C)	88% (350 °C - 720°C)	88% (720 °C - 900°C)	350
	d	3% (50 °C - 350°C)	83% (350 °C - 550°C)	83% (550 °C - 900°C)	320
Ti	**a**	5% (50 °C - 275°C)	98% (275 °C - 700°C)	98% (700 °C - 900°C)	275
	b	5% (50 °C - 400°C)	90% (340 °C - 700°C)	90% (700 °C - 900°C)	340
	c	7% (50 °C - 265°C)	95% (265 °C - 785°C)	95% (785 °C - 900°C)	265
	d	3% (50 °C - 250°C)	90% (250 °C - 700°C)	90% (700 °C - 900°C)	250
Mn	**a**	1% (50 °C - 350°C)	89% (350 °C - 850°C)	89% (850 °C - 900°C)	350
	b	3% (50 °C - 315°C)	90% (315 °C - 780°C)	90% (780 °C - 900°C)	315
	c	5% (50 °C - 300°C)	80% (300 °C - 570°C)	83% (570 °C - 900°C)	300
	d	5% (50 °C - 320°C)	98% (320 °C - 630°C)	98% (630 °C - 900°C)	320

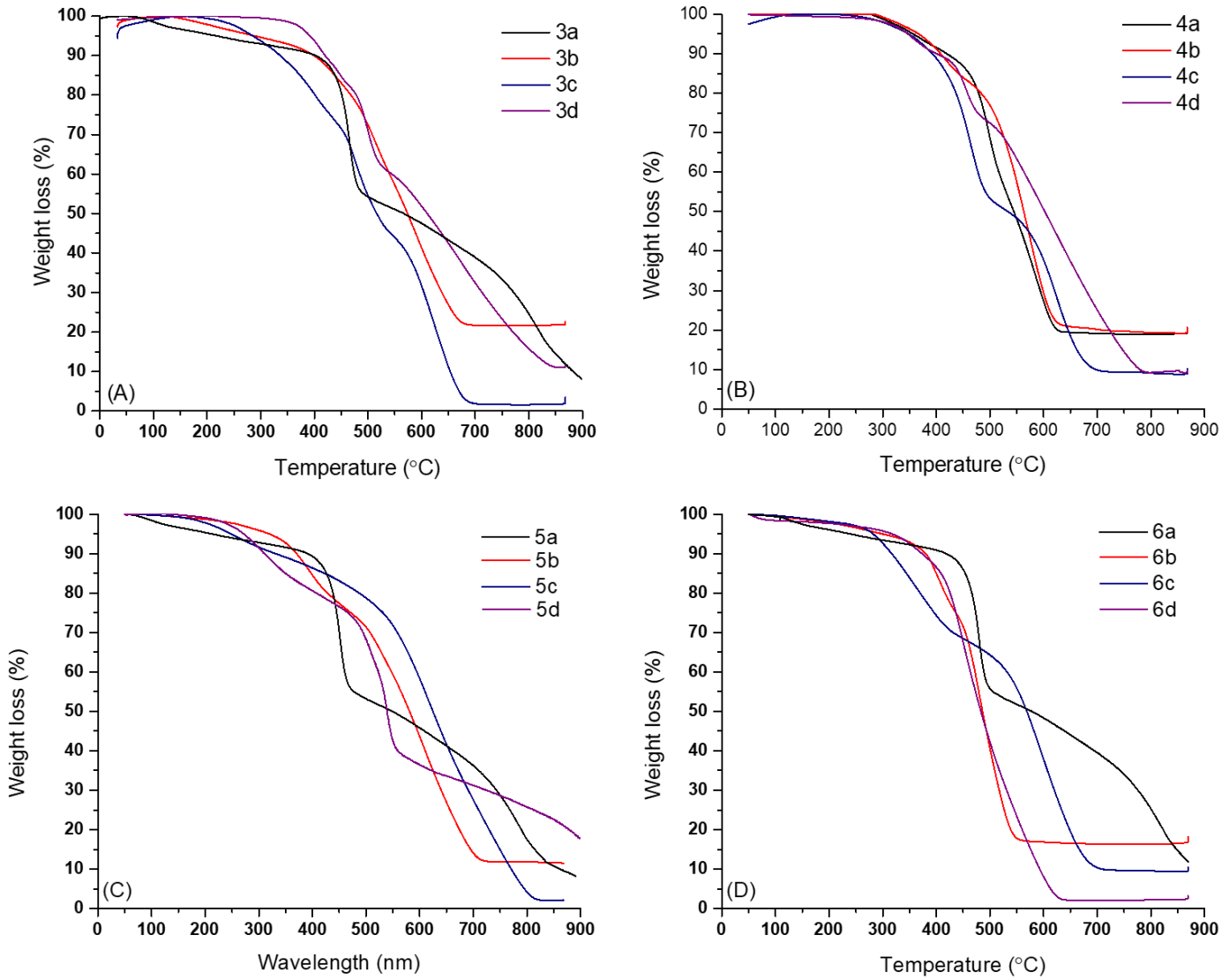


Figure S21. Thermogravimetric curves for the MPc complexes **(3a-3d, 4a-4d, 5a-5d** and **6a-6d)**.

(h) Bulk heterojunction solar cell fabrication

The BHJ cells in this work were constructed in a typical inverted configuration as follows:

Glass/ITO/comp-TiO_2/$PC_{70}BM$/MPc/P3HT/WO_3/Ag

In the inverted configuration, the photogenerated electrons are collected through the TiO_2 layer towards the ITO while the holes are collected through the WO_3 layer towards the Ag anode. The respective top and side views of the inverted BHJ cells can be viewed in Figure S22. The OSCs were fabricated on pre-cut 14 x 14 mm ITO coated glass substrates. The ITO substrates were chemically etched to remove an ~3 mm strip of ITO to reveal the underlying glass.

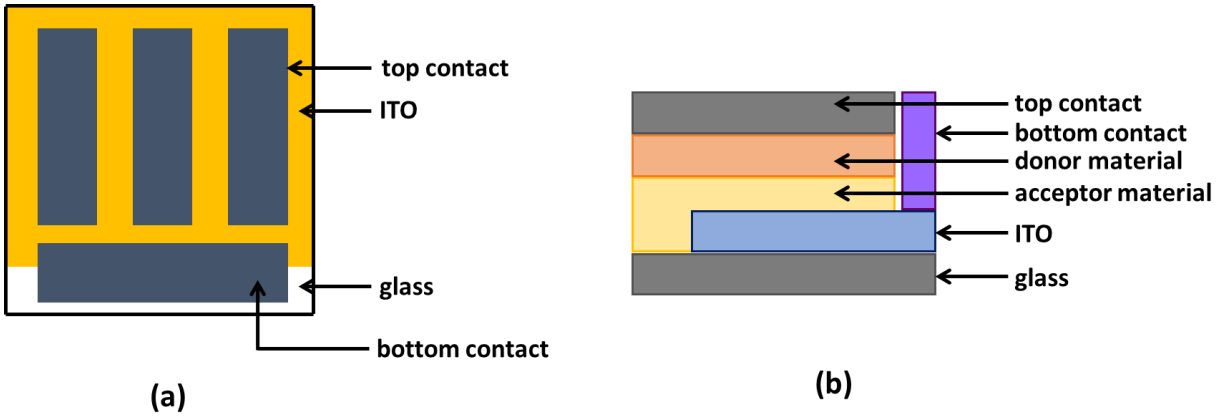


Figure S22. Top view (a) and side view (b) of the fabricated inverted BHJ OSC.

The top view shows the top and bottom contacts. Each top contact represents an individual cell or " pixel" with an active area of 0.133 cm^2. The single bottom contact lies perpendicular to the top contacts and functions the same for all three pixels. When illuminated, only the active cell area is exposed to the incoming light while the rest of the device is covered with a mask.

- *Cleaning and cutting of ITO substrates*

Commercially available ITO coated glass substrates were pre-cut into four 14 mm x 56 mm pieces and fitted onto a mask. Approximately 3 mm of the ITO length was left exposed for etching whilst the remainder of the ITO was protected by Kapton tape. The ITO substrates were chemically etched using a 2M HCl solution and Zn powder. Once etched, the ITO substrates were cut further into 14 mm x 14 mm pieces and subjected to several 5-minute cleaning cycles in an ultrasonic bath with neutral detergent, deionised water, acetone and finally IPA. The substrates were dried under a stream of N_2 flow and after that exposed to oxygen plasma treatment for 7-minutes to remove organic residue.

- *Spin coating of the ETL*

In an N_2 filled glove box, a compact TiO_2 layer was spin-coated (50 µL, 5000 rpm; 2000 m s^{-2} acceleration; 30 seconds) onto the ITO substrates. The TiO_2 coated ITO substrates were then annealed using the following temperature profile: 15-minute ramp to 450°C; 15-minute hold at 450°C; cool to 120 °C in 120 minutes.

- *Preparation and spin coating of the ternary blend photoactive layer*

Individual P3HT (30.0 mg L^{-1}), $PC_{70}BM$ (24.0 mg mL^{-1}) and MPc (10 mg mL^{-1}) solutions were prepared in chlorobenzene with stirring at 70 °C for 60 minutes in sealed vessels. The binary blend was prepared by combining the heated P3HT and $PC_{70}BM$ solutions in a 1:1.2 ratio. For the optimisation studies, MPcs **3a, 5a** and **6a** were added to the binary blend in various ratios as specified in Table S9 to form the ternary blend.

Table S9: Varying ratios of MPc for optimisation in the P3HT:$PC_{70}BM$ active layer.

Sample	**Blend ratio**		
	P3HT	**$PC_{70}BM$**	**MPc**
Reference	1	1.2	0
5 wt%	1	1.2	0.05
10 wt%	1	1.2	0.10
15 wt%	1	1.2	0.15

The ternary blends were allowed to stir at 70 °C for 30 minutes in sealed vessels. The triple blended active layer (30 µL) was deposited onto pre-heated TiO_2 coated ITO substrates *via* spin coating (800 rpm; 500 m s^{-2} acceleration; 120 seconds).

- *Thermal evaporation of HTM and anode*

Prior to the thermal deposition, the OSCs were fitted into a metal holder and covered with a shadow mask. Under vacuum conditions, a 3 nm WO_3 HTM layer followed by a 100 nm Ag layer was thermally evaporated onto the active layer, respectively. The OSCs were subjected to a final annealing step at 110 °C for 10 minutes.

- *Current-Voltage (IV-) characterization*

Standard test conditions (100 mW cm^2 under air mass, AM 1.5 global at 289 K) were applied during the measurements. The solar cells were placed into a sample holder designed to connect the bottom and top electrodes of the device to the source meter *via* gold pins. A Keithley 2400 source meter swept the bias voltage (V) from -0.1 V to 0.8 V and simultaneously monitored the corresponding current (I). A 10mV voltage step size was used and the acquisition time for one data point was set at 10 ms. A 150W Xe-lamp in a LOT Oriel solar simulator was used to simulate the AM 1.5 global standard conditions. To meet these conditions, the setup was calibrated with a certified silicon solar cell (Fraunhofer ISE WPVS Cell) equipped with a KG5 bandpass filter. The filters can reduce errors associated with the spectral mismatch between silicon and organic photovoltaic devices.

- *External quantum efficiency (EQE) characterization*

During EQE measurements, the solar cells were kept at short circuit conditions and corresponding I_{SC} were measured using a Keithley 2400 source meter. The illumination wavelength was swept from 350 nm to 950 nm in 2 nm steps. A 150W Xe-lamp in a LOT-Oriel Omni 150 monochromator equipped with a 150 nm grating, focused the monochromatic light beam onto the active cell area. A motorized filter wheel with a series of cut-of filters intersected the beam path to minimize sample radiation caused by second harmonics passing the grating monochromator. A motorized translation stage (Thorlabs PT1-Z7) was used to measured three pixels simultaneously. The incident light intensity for these measurements were calibrated with a certified silicon reference solar cell (ISE WPVS Cell, Frauenhofer Institute) with the respective KG5 filter.

(i) UV-vis spectroscopy: Optimisation of MPc concentration

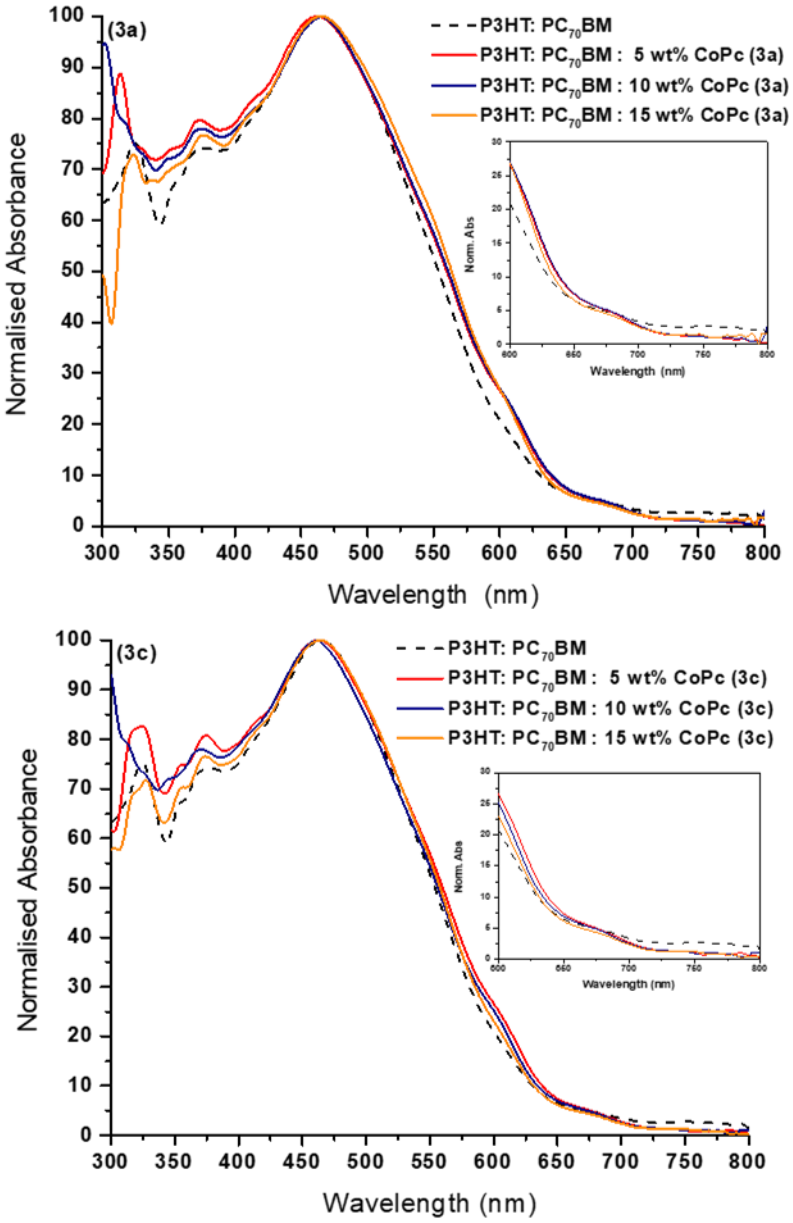


Figure S23. UV-vis spectra of CoPc complexes **(3a** and **3c)** for optimisation studies.

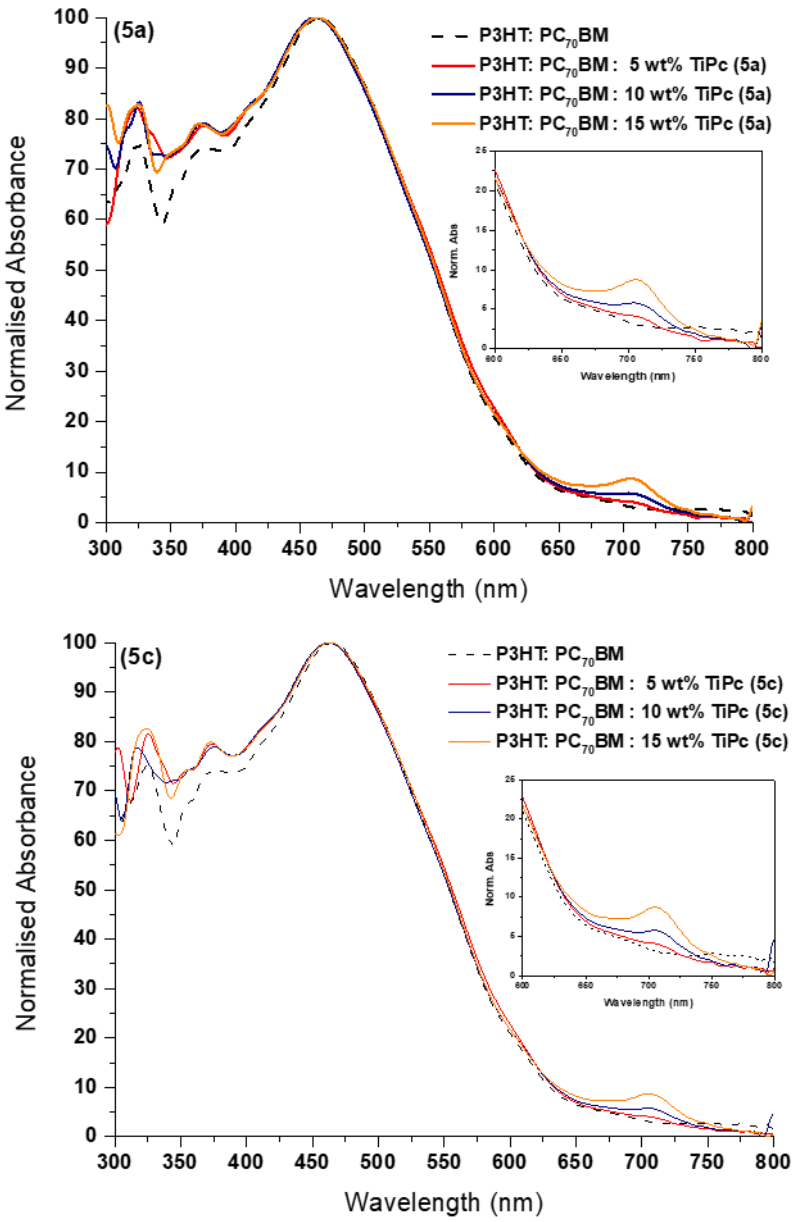


Figure S24. UV-vis spectra of TiPc complexes **(5a** and **5c)** for optimisation studies.

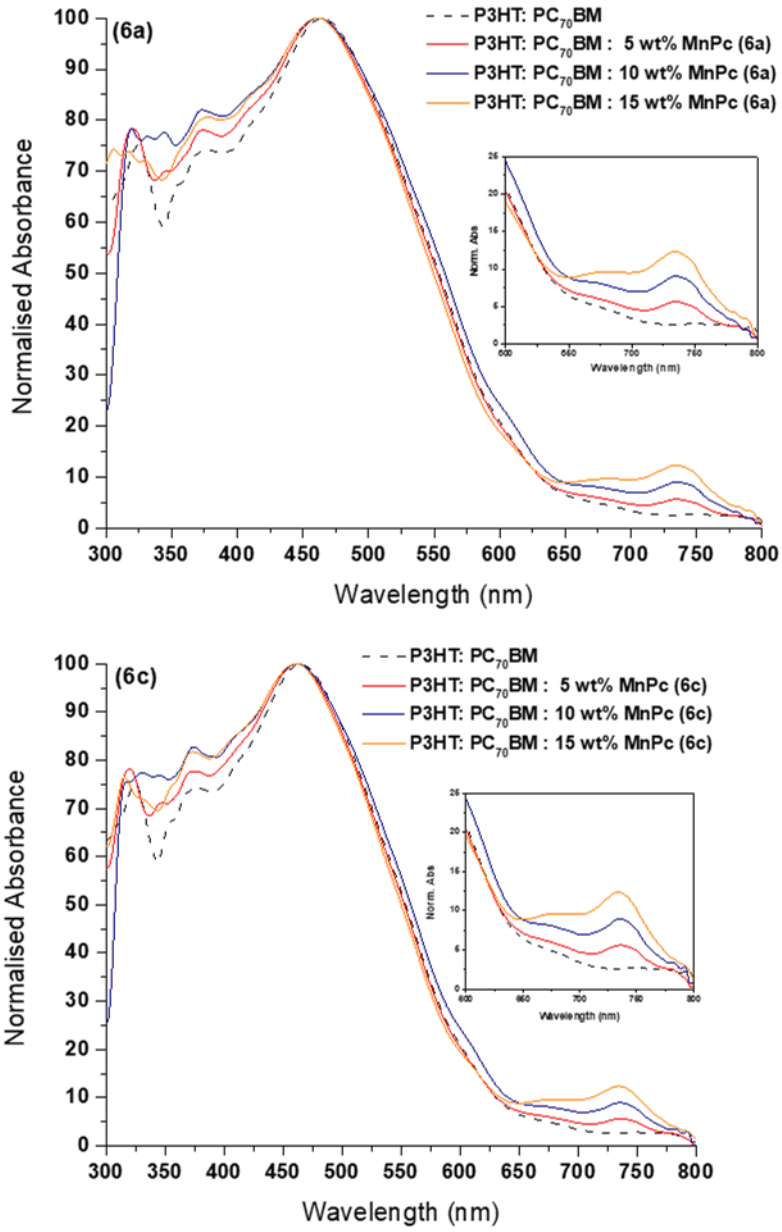


Figure S25. UV-vis spectra of MnPc complexes **(6a** and **6c)** for optimisation studies.

(j) Reverse J-V curve scans

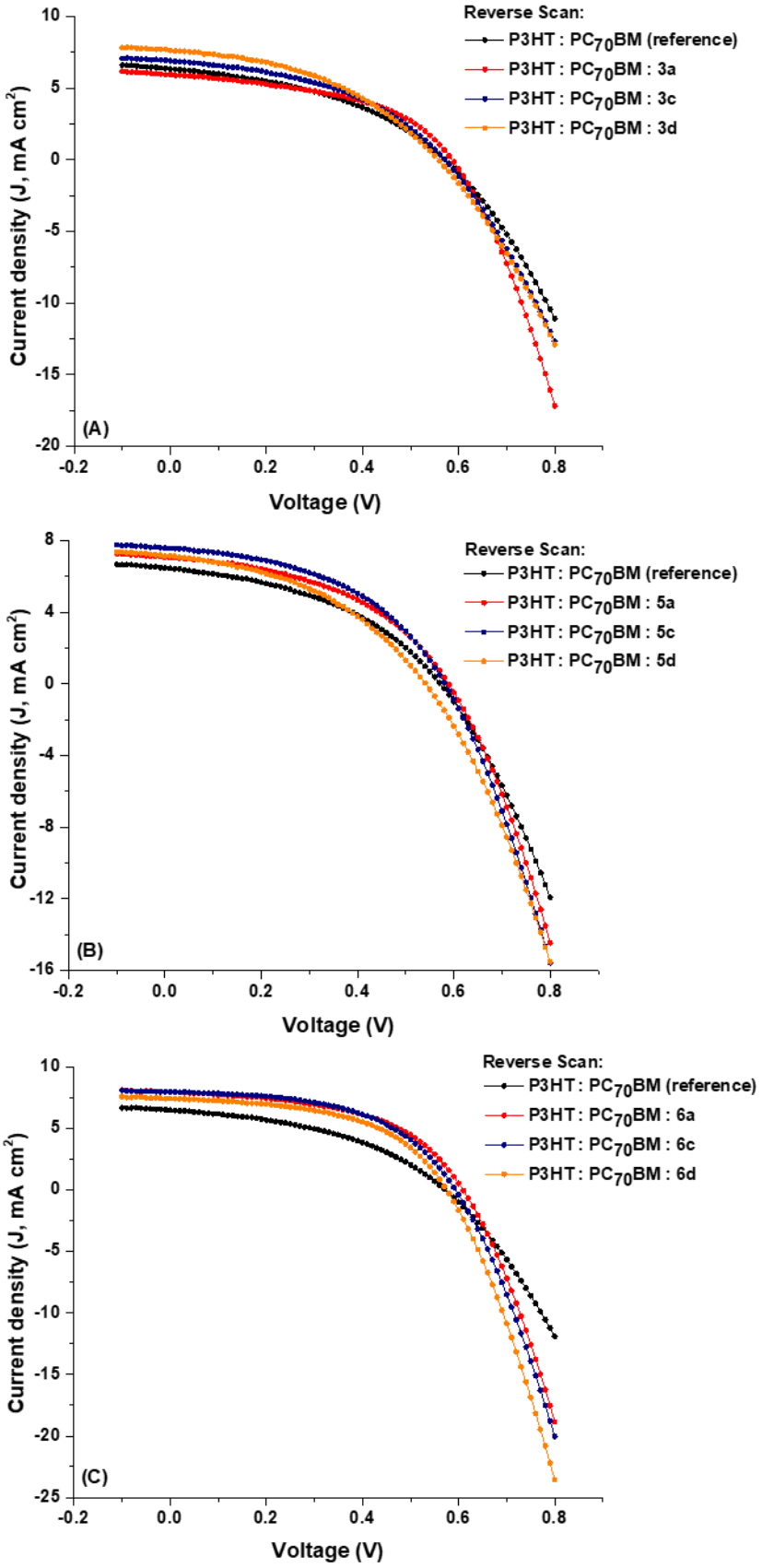


Figure S26. J-V curves (reverse scans) of BHJ OSCs with ternary components (A) **3a, 3c, 3d,** (B) **5a, 5c, 5d** and (C) **6a, 6c, 6d**.

(k) Performance parameters for reverse J-V curve scans: J_{SC}, V_{OC}, FF and PCE

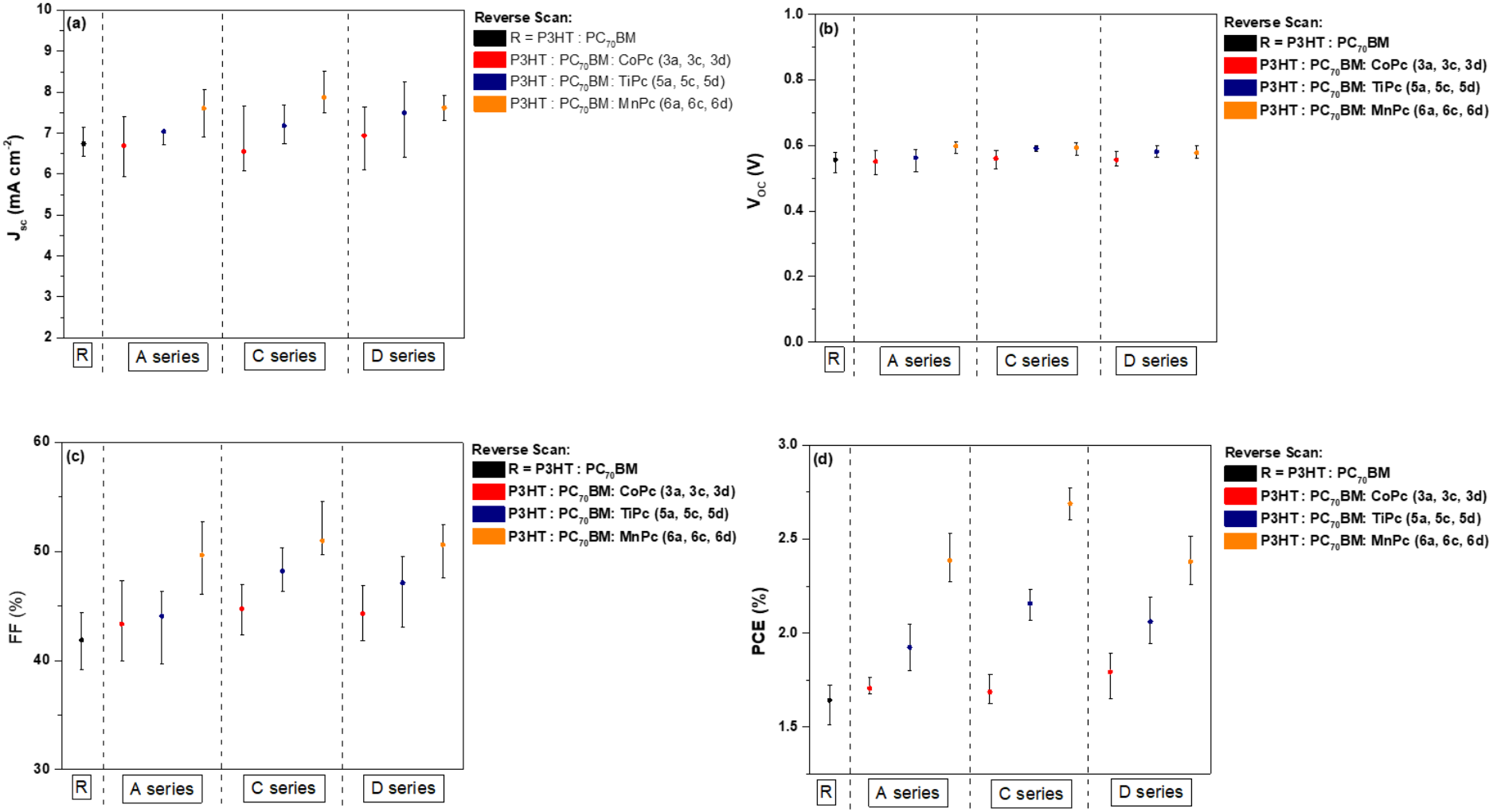


Figure S27. Comparative graphs (reverse scans) for performance parameters (a) J_{SC}, (b) V_{OC} (c) FF and (d) PCE of BHJ OSCs with MPcs **(3a, 3c, 3d, 5a, 5c, 5d** and **6a, 6c, 6d)** as ternary components.

(k) Forward and Reverse J-V curve scans

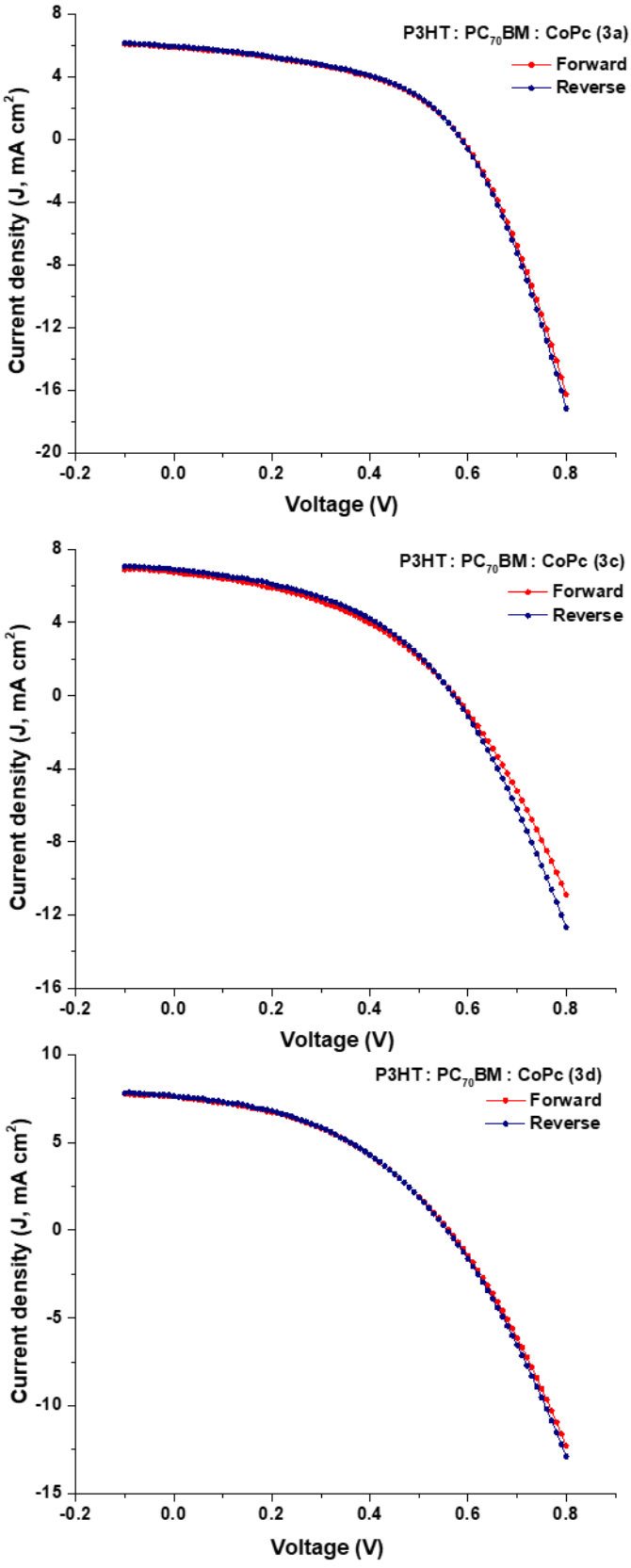


Figure S28. J-V curves (forward and reverse scans) of BHJ OSCs with CoPc **(3a, 3c, 3d)** ternary components.

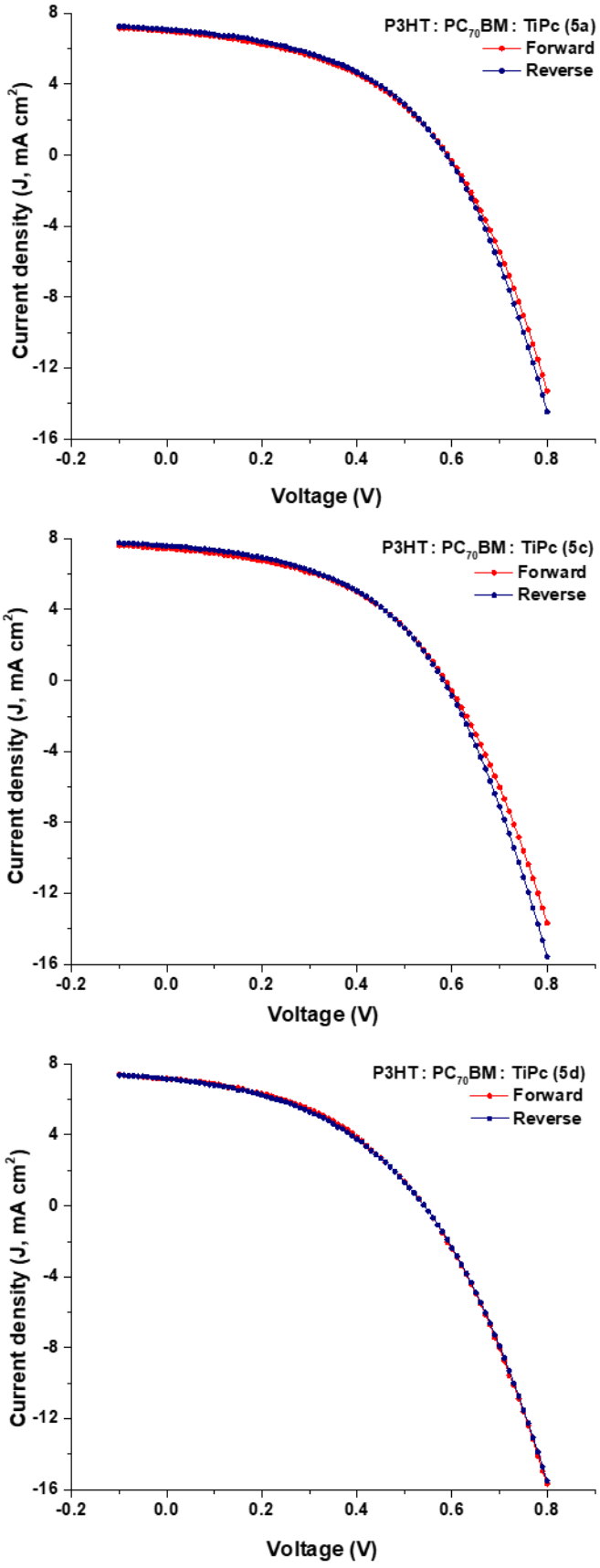
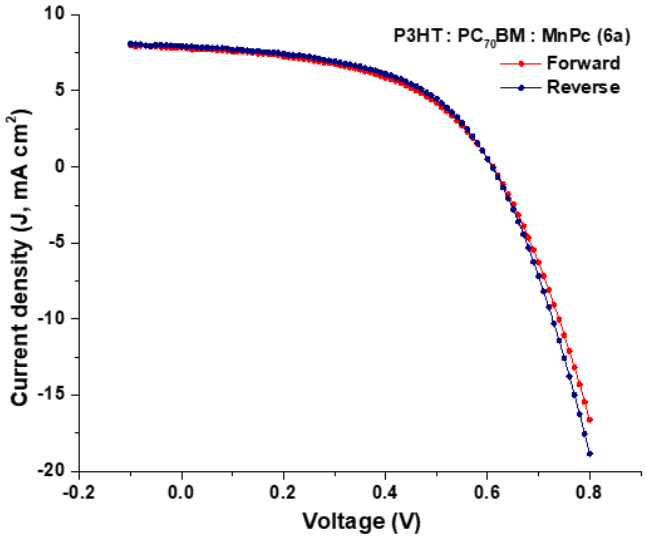
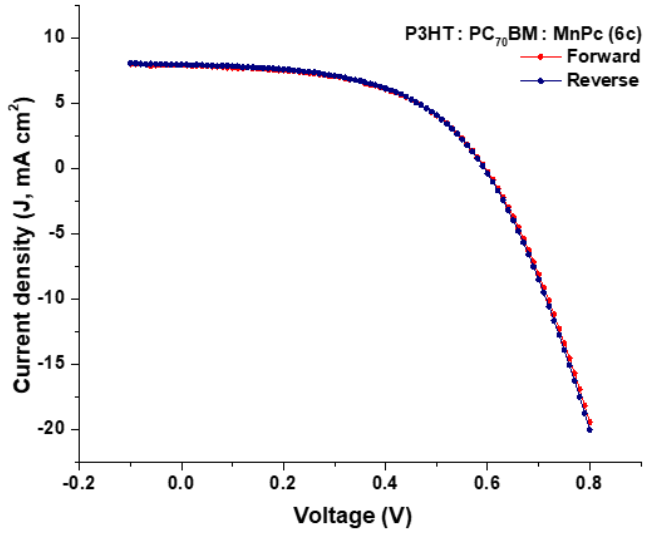


Figure S29. J-V curves (forward and reverse scans) of BHJ OSCs with TiPc **(5a, 5c, 5d)** ternary components.





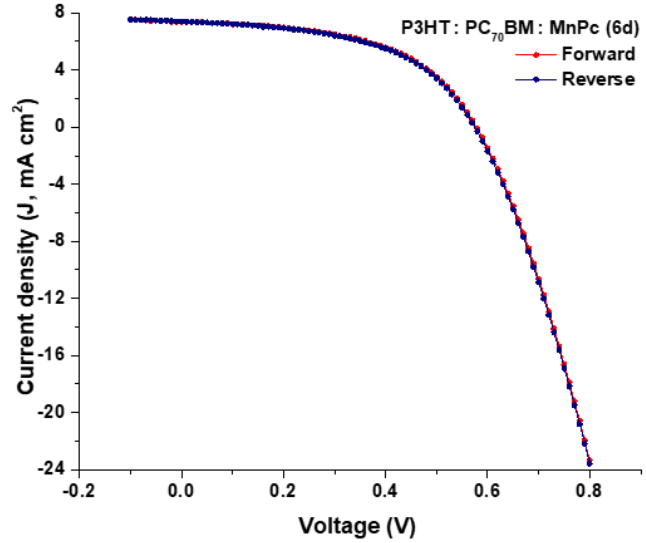


Figure S30. J-V curves (forward and reverse scans) of BHJ OSCs with MnPc **(6a, 6c, 6d)** ternary components.