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Supplementary information

A Machine Learning Approach for In-Silico Prediction of Photovoltaic Properties of Perovskite Solar Cells Based on Dopant-Free Hole-Transporting Materials

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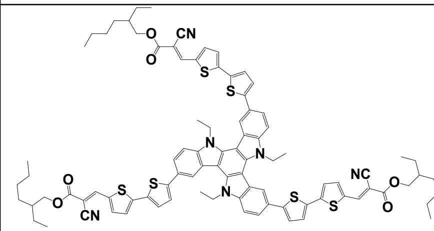
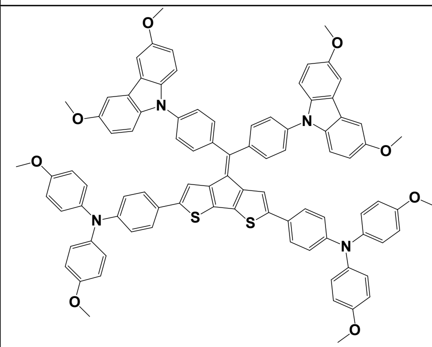
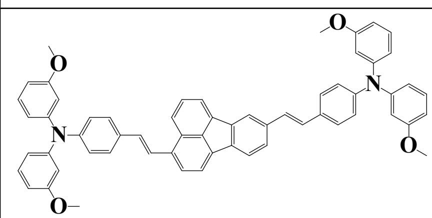
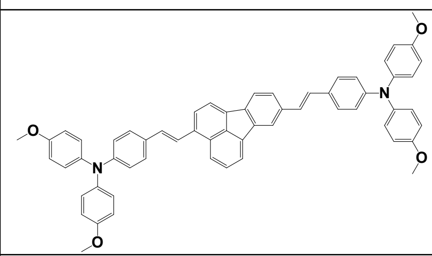
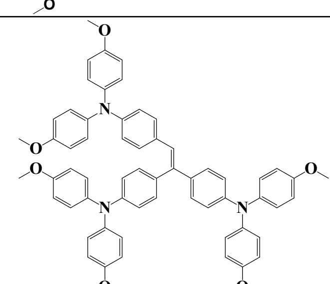
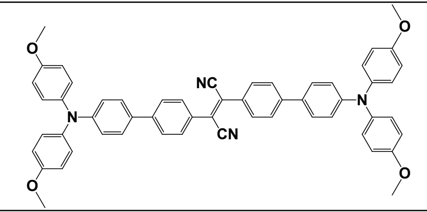
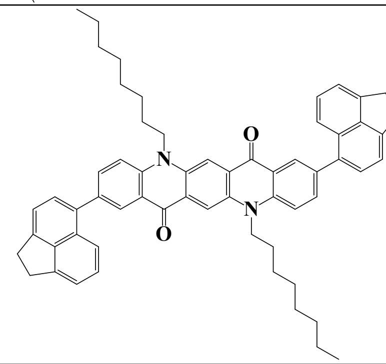
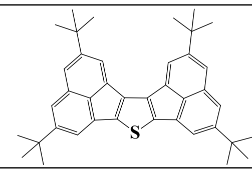
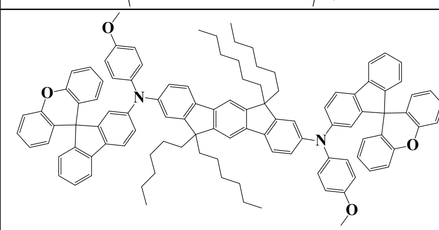
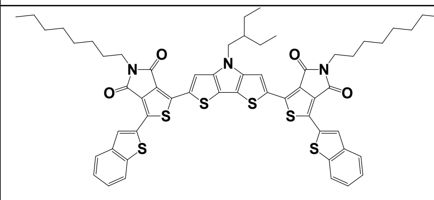
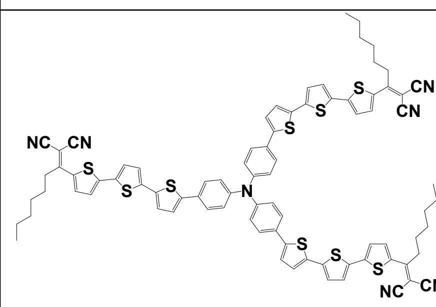
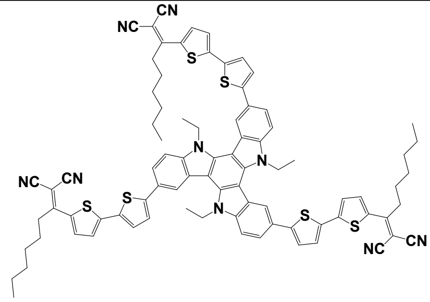
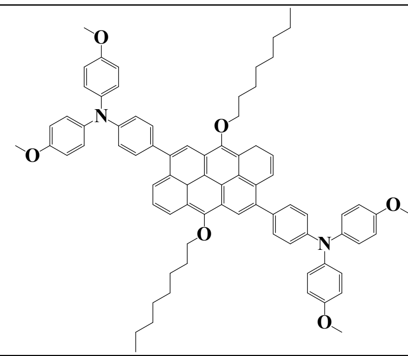
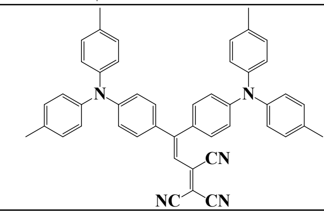
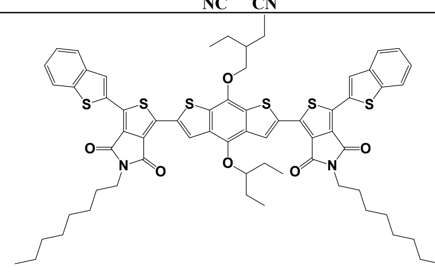
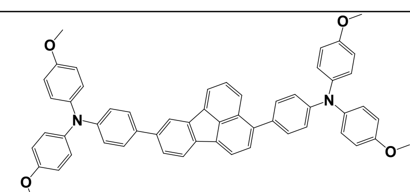
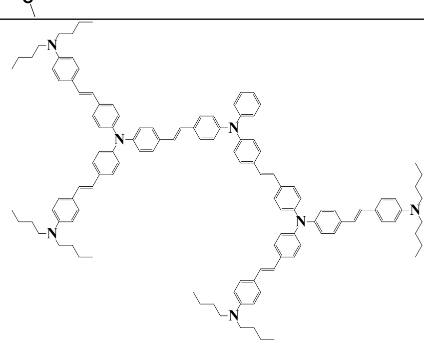
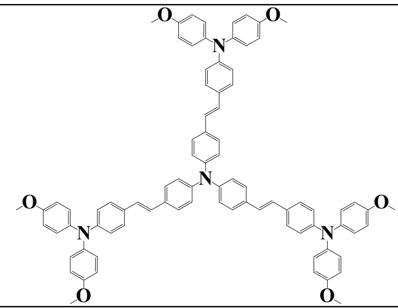
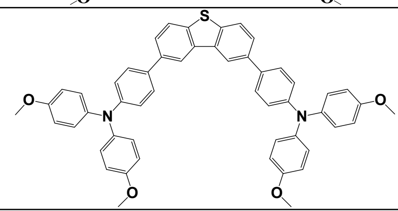
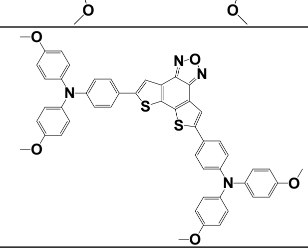
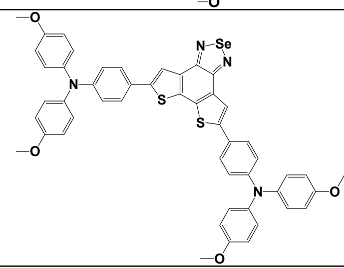
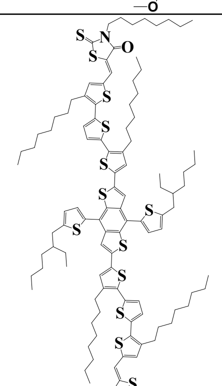
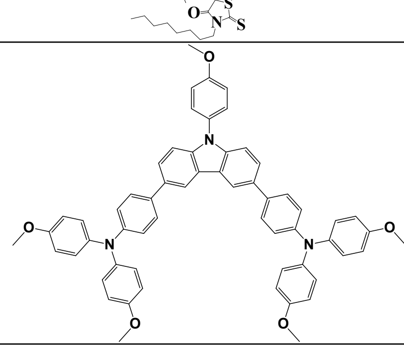
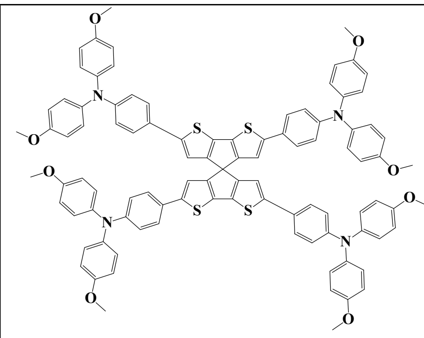
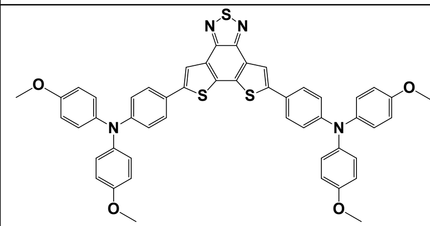
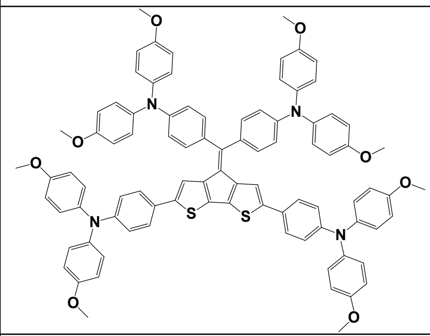
Table S1: Photovoltaic properties of dopant-free HTMs fabricated in methylammonium lead halide-based PSCs for conventional (n-i-p) and inverted (p-i-n) devices.

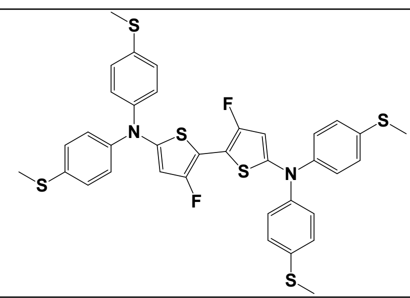
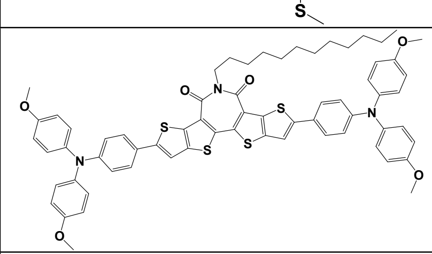
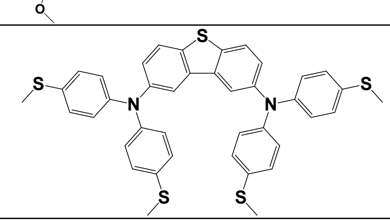
HTM	Device	Voc [V]	Jsc [mAcm^{-2}]	FF [%]	PCE [%]	Structure	Smiles
TAT–2T–CNA	ITO/SnO$_x$/PCBA/MAPbI$_3$/HTM/VO$_x$/Ag	1.13	23.1	78.0	20.1		CCN(C1=C2C=C(C3=CC=C(C4=CC=C(/C=C(C#N)/C(OCC(CCCC)CC)=O)S4)S3)C=C1)C5=C2C(N(CC)C6=C7C=C(C8=CC=C(C9=CC=C(/C=C(C#N)/C(OCC(CCCC)CC)=O)S9)S8)C=C6)=C7C%10=C5C%11=C(C=CC(C%12=CC=C(C%13=CC=C(/C=C(C#N)/C(OCC(CCCC)CC)=O)S%13)S%12)=C%11)N%10CC
C-CPDT	FTO/c-TiO$_2$/mp-TiO$_2$/MAPbI$_3$/HTM/Ag	1.14	23.27	74.2	19.6		COC(C=C12)=CC=C1N(C3=C2C=C(OC)C=C3)C(C=C4)=CC=C4/C(C5=CC=C(N(C6=CC=C(OC)C=C67)C8=C7C=C(OC)C=C8)C=C5)=C9C%10=C(SC(C%11=CC=C(N(C%12=CC=C(OC)C=C%12)C%13=CC=C(OC)C=C%13)C=C%11)=C%10)C%14=C\9C=C(C%15=CC=C(N(C%16=CC=C(OC)C=C%16)C%17=CC=C(OC)C=C%17)C=C%15)S%14
FBA3	ITO/C$_{60}$/MAPbI$_x$Cl$_{3_x}$/HTM/MoO$_3$/Ag	1.09	22.12	0.799	19.27		COC1=CC(N(C2=CC(OC)=CC=C2)C(C=C3)=CC=C3/C=C/C4=CC=C5C6=C4C=CC=C6C7=C5C=CC(/C=C/C8=CC=C(N(C9=CC(OC)=CC=C9)C%10=CC(OC)=CC=C%10)C=C8)=C7)=CC=C1
FBA2	ITO/C$_{60}$/Cl$_{3_x}$/MAPbI$_x$/HTM/MoO$_3$/Ag	1.06	22.32	79.0	18.7		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(/C=C/C(C=C4)=CC5=C4C6=CC=C(/C=C/C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)C%10=C6C5=CC=C%10)C=C3
CJ-01	FTO/TiO$_2$/meso-TiO$_2$/MAPbI$_3$/HTM/Au	1.113	22.32	0.747	18.56		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(/C(C4=CC=C(N(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)C=C4)=C/C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)C=C3

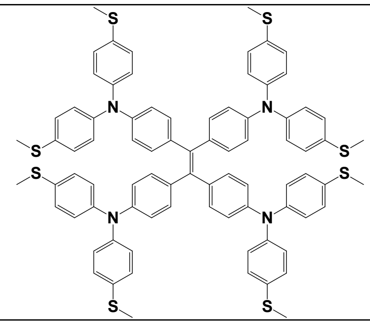
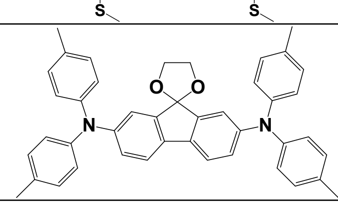
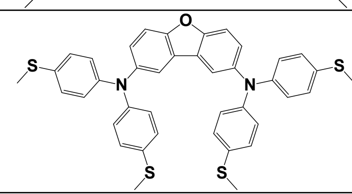
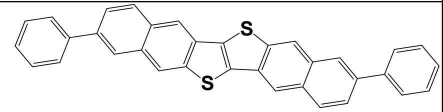
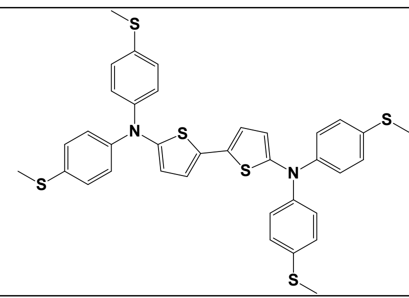
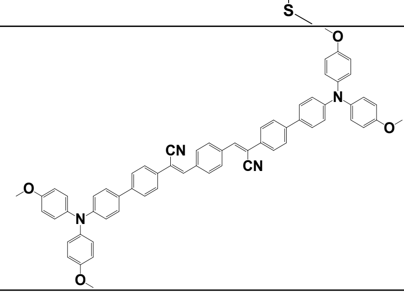
TPA–BPFN–TPA	FTO/c-TiO_2/m-TiO_2/$MAPbI_3$/HTM/Ag	1.04	22.70	78.0	18.4		N#C/C(C1=CC=C(C2=CC=C(N(C3=CC=C(OC)C=C3)C4=CC=C(OC)C=C4)C=C2)C=C1)=C(C#N)\C(C=C5)=CC=C5C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6
ACE-QA-ACE	FTO/TiO_2/meso-TiO_2/$MAPbI_3$/HTM/Ag	1.06	22.41	0.77	18.2		O=C1C2=C(C=C(C(C(C=C(C3=CC=C4C5=C3C=CC=C5CC4)C=C6)=C6N7CCCCCCCC)=O)C7=C2)N(CCCCCCCC)C8=CC=C(C9=CC=C%10C%11=C9C=CC=C%11CC%10)C=C81
PCA-1	FTO/TiO_2/meso-TiO_2/$MAPbI_3$/HTM/Au	1.062	22.3	0.767	18.17		CC(C)(C)C1=CC2=CC(C(C)(C)C)=CC(C3=C4C(C5=CC(C(C)(C)C)=CC6=CC(C(C)(C)C)=CC7=C56)=C7S3)=C2C4=C1
IDF-SFXPh	FTO/C_{60}/$MAPbI_{3\_x}Cl_x$/HTM/MoO_3/Ag	1.05	21.5	0.773	17.6		COC(C=C1)=CC=C1N(C2=CC(C3(C(C=CC=C4)=C4OC5=C3C=CC=C5)C6=C7C=CC=C6)=C7C=C2)C8=CC(C9(CCCCCC)CCCCCC)=C(C=C8)C(C9=C%10)=CC%11=C%10C(C=CC(N(C%12=CC(C%13(C(C=CC=C%14)=C%14OC%15=C%13C=CC=C%15)C%16=C%17C=CC=C%16)=C%17C=C%12)C%18=CC=C(OC)C=C%18)=C%19)=C%19C%11(CCCCCC)CCCCCC
BTDTP	FTO/c-TiO_2/m-TiO_2/$MAPbI_3$/BTDTP/Ag	0.97	25.73	70.5	17.6		O=C(N1CCCCCCCC)C2=C(C3=CC(C=CC=C4)=C4S3)SC(C(S5)=CC6=C5C(SC(C7=C(C(N(CCCCCCCC)C8=O)=O)C8=C(C9=CC%10=C(C=CC=C%10)S9)S7)=C%11)=C%11N6CC(CC)CC)=C2C1=O
TPA–3T–DCV	ITO/SnO_x/PCBA/$MAPbI_3$/HTM/**VO_x**/Ag	1.08	23.0	71.0	17.6		CCCCCC/C(C1=CC=C(S1)C(S2)=CC=C2C3=CC=C(S3)C4=CC=C(N(C5=CC=C(C6=CC=C(C7=CC=C(C8=CC=C(/C(CCCCCC)=C(C#N)\C#N)S8)S7)S6)C=C5)C9=CC=C(C%10=CC=C(C%11=CC=C(C%12=CC=C(/C(CCCCCC)=C(C#N)/C#N)S%12)S%11)S%10)C=C9)C=C4)=C(C#N)/C#N

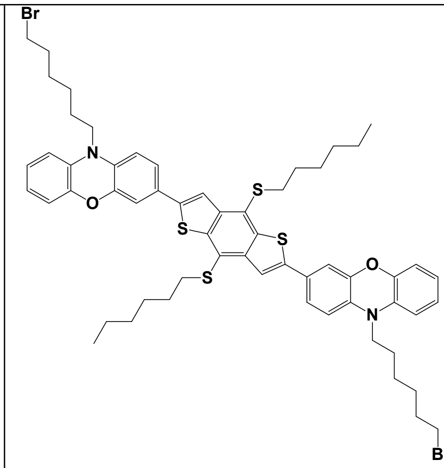
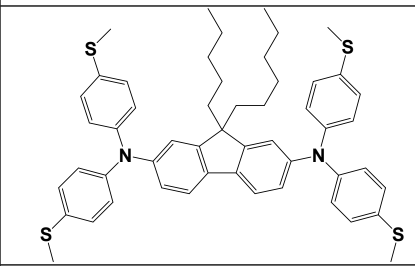
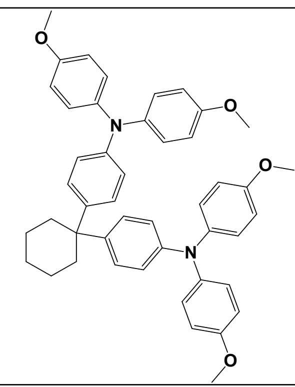
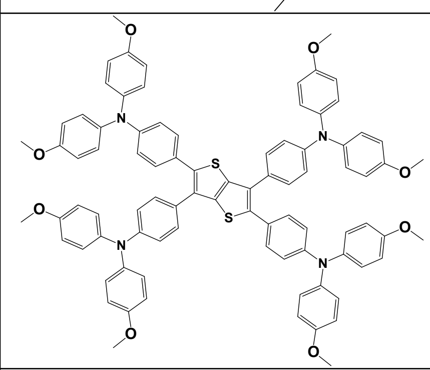
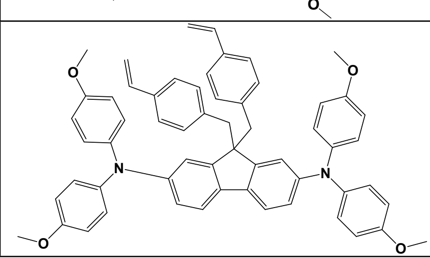
TAT–2T–DCV	ITO/SnO_x/PCBA/$MAPbI_3$/HTM/VO_x/Ag	1.08	23.0	71.0	17.6		CCN(C1=C2C=C(C3=CC=C(C4=CC=C(/C(CCCCCC)=C(C#N)\C#N)S4)S3)C=C1)C5=C2C(N(CC)C6=C7C=C(C8=CC=C(C9=CC=C(/C(CCCCCC)=C(C#N)/C#N)S9)S8)C=C6)=C7C%10=C5C%11=C(C=CC(C%12=CC=C(C%13=CC=C(/C(CCCCCC)=C(C#N)/C#N)S%13)S%12)=C%11)N%10CC
TPA-ANT-TPA	FTO/TiO_2/meso-TiO_2/$MAPbI_3$/HT/Ag	1.03	21.07	0.796	17.5		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC5=C6C(C(C7=C5OCCCCCCCC)=C(C=CC7)C(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)=C%11)=C%11C(OCCCCCCCC)=C%12C6C4=CC=C%12
BTPA-TCNE	FTO/SnO_2/PCBM/$MAPbI_3$/HTM/MoO_3/Au	1.04	20.84	0.782	16.94		CC(C=C1)=CC=C1N(C2=CC=C(C)C=C2)C3=CC=C(/C(C4=CC=C(N(C5=CC=C(C)C=C5)C6=CC=C(C)C=C6)C=C4)=C\C(C#N)=C(C#N)\C#N)C=C3
BTBDT	FTO/c-TiO_2/$MAPbI_3$/m-TiO_2/BTDTP/Ag	0.95	24.68	72.3	16.9		O=C(N1CCCCCCCC)C2=C(C3=CC(C=CC=C4)=C4S3)SC(C5=CC6=C(C(OCC(CC)CC)=C7SC(C8=C(C(N(CCCCCCCC)C9=O)=O)C9=C(C%10=CC%11=C(C=CC=C%11)S%10)S8)=CC7=C6OC(CC)CC)S5)=C2C1=O
FBA1	ITO/C_{60}/$MAPbI_x/Cl_{3-x}$/HTM/MoO_3/Ag	1.05	21.57	74.2	16.8		COC1=CC=C(N(C2=CC=C(C3=CC=C4C5=C3C=CC=C5C6=C4C=C(C7=CC=C(C=C7)N(C8=CC=C(C=C8)OC)C9=CC=C(C=C9)OC)C=C6)C=C2)C%10=CC=C(C=C%10)OC)C=C1
Z1011	FTO/TiO_2/meso-TiO_2/$MAPbI_3$/HTM/Au	1.096	20.52	0.7	16.3		CCCCN(CCCC)C(C=C1)=CC=C1/C=C/C(C=C2)=CC=C2N(C3=CC=C(/C=C/C4=CC=C(N(CCCC)CCCC)C=C4)C=C3)C5=CC=C(/C=C/C6=CC=C(N(C7=CC=CC=C7)C8=CC=C(/C=C/C9=CC=C(N(C%10=CC=C(/C=C/C%11=CC=C(N(CCCC)CCCC)C=C%11)C=C%10)C%12=CC=C(/C=C/C%13=CC=C(N(CCCC)CCCC)C=C%13)C=C%12)C=C9)C=C8)C=C6)C=C5

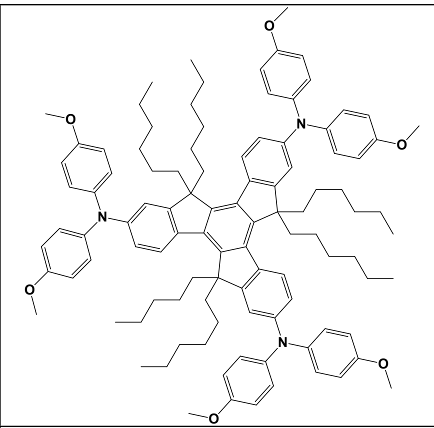
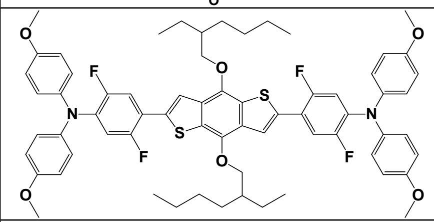
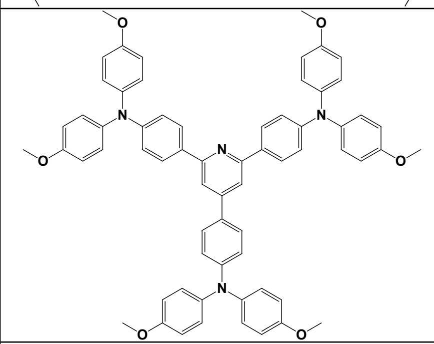
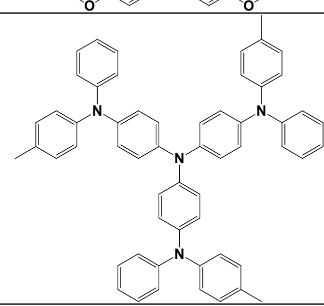
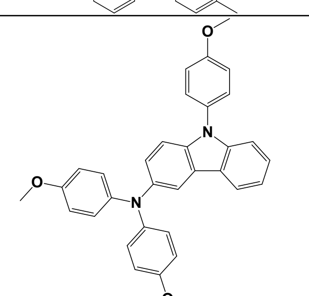
Z34	FTO/TiO_2/meso-TiO_2/$MAPbI_3$/HTM/Au	1.055	21.245	0.70	16.1		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(/C=C/C4=CC=C(N(C5=CC=C(/C=C/C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)C=C5)C9=CC=C(/C=C/C%10=CC=C(N(C%11=CC=C(OC)C=C%11)C%12=CC=C(OC)C=C%12)C=C%10)C=C9)C=C4)C=C3
CQ2	ITO/SnO_2/C_{60}/$MAPbI_{3-x}Cl_x$/HTM/MoO_3/Ag	1.02	20.57	72.6	15.2		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC5=C(C=C4)SC6=C5C=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)C=C6
DTBT	ITO/SnO_2/$MAPbI_3$/HTM/MoO_3/Ag	0.93	22.20	56.1	11.6		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC5=C(S4)C6=C(C=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)S6)C%10=NON=C5%10
DTBS	ITO/SnO_2/$MAPbI_3$/HTM/MoO_3/Ag	0.96	22.78	69.1	15.0		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC5=C(S4)C6=C(C=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)S6)C%10=N[Se]N=C5%10
DOR3T-TBDT	ITO/TiO_2/$MAPbI_{3-x}Cl_x$/HTM/MoO_3/Ag	0.97	20.7	0.74	14.9		O=C(/C(S1)=C/C(S2)=CC(CCCCCCCC)=C2C3=CC=C(S3)C(S4)=C(CCCCCCCC)C=C4C5=CC6=C(C7=CC=C(CC(CCCC)CC)S7)C8=C(C=C(C9=CC(CCCCCCCC)=C(C%10=CC=C(C%11=C(CCCCCCCC)C=C(/C=C%12SC(N(CCCCCCCC)C\%12=O)=S)S%11)S%10)S9)S8)C(C%13=CC=C(CC(CCCC)CC)S%13)=C6S5)N(CCCCCCCC)C1=S
X25	ITO/SnO_2/C_{60}/ $MAPbI_{3-x}Cl_x$/ HTM/MoO_3/Ag	1.01	19.64	72.4	14.4		COC(C=C1)=CC=C1N2C(C=CC(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)=C6)=C6C7=C2C=CC(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)=C7

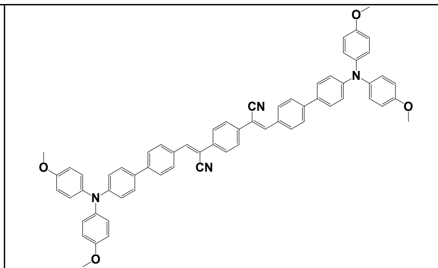
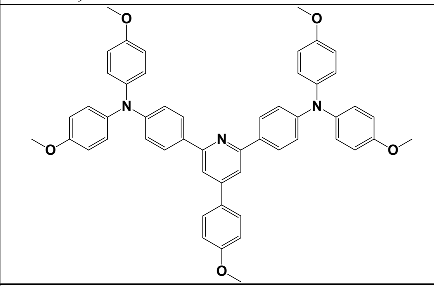
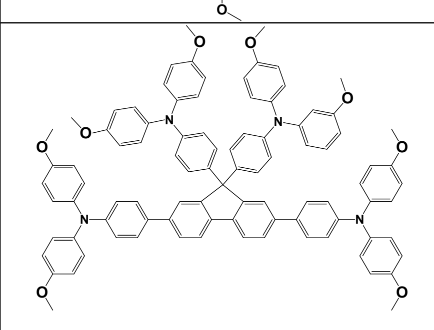
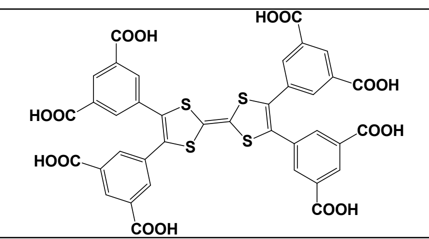
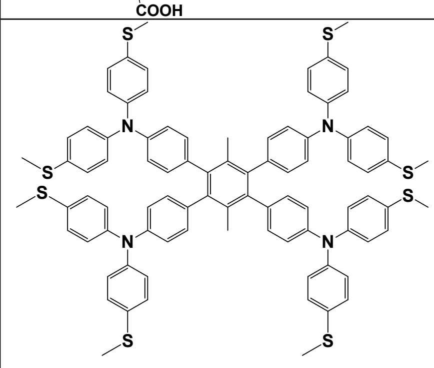
HTM 1	FTO/TiO_2/HTM/Au/$MAPbI_3$/mp-TiO_2	0.971	19.3	0.716	13.4		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC(C5(C(C=C(C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)S9)=C9C%10=C5C=C(C%11=CC=C(N(C%12=CC=C(OC)C=C%12)C%13=CC=C(OC)C=C%13)C=C%11)S%10)C%14=C%15SC(C%16=CC=C(N(C%17=CC=C(OC)C=C%17)C%18=CC=C(OC)C=C%18)C=C%16)=C%14)=C%15S4
DTBF	ITO/SnO_2/$MAPbI_3$/HTM/MoO_3/Ag	0.95	22.48	62.3	13.3		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC5=C(S4)C6=C(C=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)S6)C%10=NSN=C5%10
T-CPDT	FTO/c-TiO_2/mp-TiO_2/$MAPbI_3$/HTM/Ag	0.88	21.37	60.9	11.4		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3/C(C4=CC=C(N(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)C=C4)=C7C8=C(SC(C9=CC=C(N(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)C=C9)=C8)C%12=C\7C=C(C%13=CC=C(N(C%14=CC=C(OC)C=C%14)C%15=CC=C(OC)C=C%15)C=C%13)S%12

HTM	**Device configuration**	**Voc [V]**	**Jsc [mAcm^{-2}]**	**FF [%]**	**PCE [%]**	**Structure**	**Smiles**
DFBT–MTP	ITO/HTM/$MAPbI_{3-x}Cl_x$/C_{60}/BCP/Ag	1.16	22.15	82.2	21.2		FC1=C(C2=C(F)C=C(N(C3=CC=C(SC)C=C3)C4=CC=C(SC)C=C4)S2)SC(N(C5=CC=C(SC)C=C5)C6=CC=C(SC)C=C6)=C1
MPA-BTTI	ITO/HTM/CsFAMA/C_{60}/BCP/Ag	1.12	23.23	0.814	21.17		O=C(C1=C(C2=C3C4=C(C=C(C5=CC=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5)S4)S2)SC8=C1SC(C9=CC=C(N(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)C=C9)=C8)N(CCCCCCCCCCCC)C3=O
DBTMT	ITO/HTM/$MAPbI_3$/C_{60}/BCP/Ag	1.12	22.70	83.2	21.1		CSC(C=C1)=CC=C1N(C2=CC=C(SC)C=C2)C3=CC=C4C(C5=C(S4)C=CC(N(C6=CC=C(SC)C=C6)C7=CC=C(SC)C=C7)=C5)=C3

TPE-S	ITO/TPE-S/$Cs_{0.1}FA_{0.9}PbI_3$/PCBM/ZnO/Ag	1.13	23.3	0.797	21		CSC(C=C1)=CC=C1N(C2=CC=C(SC)C=C2)C(C=C3)=CC=C3/C(C4=CC=C(N(C5=CC=C(SC)C=C5)C6=CC=C(SC)C=C6)C=C4)=C(C7=CC=C(N(C8=CC=C(SC)C=C8)C9=CC=C(SC)C=C9)C=C7)/C%10=CC=C(N(C%11=CC=C(SC)C=C%11)C%12=CC=C(SC)C=C%12)C=C%10
DFH	ITO/HTM/$MA_{0.9}FA_{0.1}PbI_{3\_x}Cl_x$/$C_{60}$/BCP/Ag	1.09	22.7	0.83	20.6		CC(C=C1)=CC=C1N(C2=CC=C(C)C=C2)C(C=C3C45OCCO5)=CC=C3C6=C4C=C(N(C7=CC=C(C)C=C7)C8=CC=C(C)C=C8)C=C6
DBFMT	ITO/HTM/$MAPbI_3$/C_{60}/BCP/Ag	1.07	23.70	80.4	20.5		CSC(C=C1)=CC=C1N(C2=CC=C(SC)C=C2)C3=CC=C4C(C5=C(O4)C=CC(N(C6=CC=C(SC)C=C6)C7=CC=C(SC)C=C7)=C5)=C3
DPh–DNTT	ITO/HTM/$MAPbI_3$/$PC_{61}BM$/BCP/Ag	1.10	22.56	80.0	20.1		C1(C(C=C(C=CC(C2=CC=CC=C2)=C3)C3=C4)=C4S5)=C5C(C=C(C=CC(C6=CC=CC=C6)=C7)C7=C8)=C8S1
BT–MTP	ITO/HTM/$MAPbI_{3\_x}Cl_x$/C_{60}/BCP/Ag	1.10	23.01	79.7	20.1		CSC(C=C1)=CC=C1N(C2=CC=C(SC)C=C2)C3=CC=C(S3)C4=CC=C(N(C5=CC=C(SC)C=C5)C6=CC=C(SC)C=C6)S4
YJ01	ITO/HTM/$MAPbI_3$/PC61BM/BCP/Ag	1.08	22.53	81.5	19.8		N#C/C(C1=CC=C(C2=CC=C(N(C3=CC=C(OC)C=C3)C4=CC=C(OC)C=C4)C=C2)C=C1)=C\C5=CC=C(/C=C(C#N)/C6=CC=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)C=C6)C=C5

BDT-POZ	ITO/HTM/MAPbI_3/PCBM/BCP/Ag	1.04	22.56	0.817	19.16		BrCCCCCCN(C(C=CC=C1)=C1O2)C(C2=C3)=CC=C3C(S4)=CC5=C4C(SCCCCCC)=C(C=C(C6=CC=C(N(CCCCCCBr)C(C=CC=C7)=C7O8)C8=C6)S9)C9=C5SCCCCCC
FMT	ITO/HTM/MAPbI_3/PCBM/Al	1.07	22.52	0.792	19.06		CSC(C=C1)=CC=C1N(C2=CC=C(SC)C=C2)C(C=C3C4(CCCCCC)CCCCCC)=CC=C3C5=C4C=C(N(C6=CC=C(SC)C=C6)C7=CC=C(SC)C=C7)C=C5
TAPC	ITO/HTM/MAPbI_3/PCBM/Ag	1.04	22.32	0.811	18.80		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(C4(C5=CC=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5)CCCCC4)C=C3
XY1	ITO/HTM/$Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$/$C_{60}$/BCP/Ag	1.11	22.21	0.761	18.78		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=C(C5=CC=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5)SC8=C4SC(C9=CC=C(N(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)C=C9)=C8C%12=CC=C(N(C%13=CC=C(OC)C=C%13)C%14=CC=C(OC)C=C%14)C=C%12
VB-MeO-FDPA	ITO/HTMs/Perovskite/PCBM/PEI/Ag	1.15	20.89	0.778	18.7		C=CC1=CC=C(CC2(CC3=CC=C(C=C)C=C3)C4=CC(N(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)=CC=C4C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C72)C=C1

Trux-OMeTAD	ITO/HTM/MAPbI$_3$/PCBM/ZnO NPS/Al	1.02	23.2	0.79	18.6		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC4=C3C5=C(C(CCCCCC)(CCCCCC)C6=C7C=CC(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)=C6)C7=C(C(CCCCCC)(CCCCCC)C%10=C%11C=CC(N(C%12=CC=C(OC)C=C%12)C%13=CC=C(OC)C=C%13)=C%10)C%11=C5C4(CCCCCC)CCCCCC
H2	ITO/HTM/MAPbI$_3$/PC$_{61}$BM/BCP/Ag	1.06	22.93	76.9	18.6		FC1=C(N(C2=CC=C(OC)C=C2)C3=CC=C(OC)C=C3)C=C(F)C(C(S4)=CC(C4=C5OCC(CC)CCCC)=C(OCC(CC)CCCC)C6=C5C=C(C7=CC(F)=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7F)S6)=C1
D106	ITO/HTM/MAPbI$_3$/PC$_{61}$BM/BCP/Ag	1.05	22.32	77.8	18.2		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC(C5=CC=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5)=CC(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)=N4
m-MTDATA	ITO/HTM/MAPbI/PCBM/BCP/Cu	1.035	22.5	0.78	18.12		CC(C=C1)=CC=C1N(C2=CC=CC=C2)C3=CC=C(N(C4=CC=C(N(C5=CC=C(C)C=C5)C6=CC=CC=C6)C=C4)C7=CC=C(N(C8=CC=CC=C8)C9=CC=C(C)C=C9)C=C7)C=C3
TPAC3M	ITO/HTM/MAPbI$_3$/PCBM/ZnO/Al	1.00	22.79	0.78	17.54		COC(C=C1)=CC=C1N2C3=C(C=CC=C3)C4=C2C=CC(N(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)=C4

YJ02	ITO/HTM/MAPbI$_3$/PC$_{61}$BM/BCP/Ag	1.04	22.22	75.5	17.5		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C(C=C4)=CC=C4/C=C(C#N)/C5=CC=C(/C(C#N)=C/C6=CC=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)C=C6)C=C5
D105	ITO/HTM/MAPbI$_3$/PC$_{61}$BM/BCP/Ag	1.04	21.96	76.1	17.4		COC1=CC=C(C2=CC(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)=NC(C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)=C2)C=C1
TPA-2,7-FLTPA-TPA	ITO/MoO$_3$/HTM/MAPbI$_3$/C$_{60}$/BCP/Ag	1.052	20.82	0.78	17.1		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC=C5C6=CC=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)C=C6C(C%10=CC=C(N(C%11=CC=C(OC)C=C%11)C%12=CC=C(OC)C=C%12)C=C%10)(C%13=CC=C(N(C%14=CC=CC(OC)=C%14)C%15=CC=C(OC)C=C%15)C=C%13)C5=C4
TTA	ITO/HTM/MAPbI$_3$/PCBM/C$_{60}$/BCP/Ag	1.04	20.4	0.78	16.7		O=C(O)C1=CC(C(O)=O)=CC(C2=C(C3=CC(C(O)=O)=CC(C(O)=O)=C3)S/C(S2)=C4SC(C5=CC(C(O)=O)=CC(C(O)=O)=C5)=C(C6=CC(C(O)=O)=CC(C(O)=O)=C6)S\4)=C1
TPP-SMeTAD	ITO/HTM/MAPbI$_3$/PCBM/ZnO NP$_s$/Al	1.07	20.15	0.77	16.6		CC1=C(C2=CC=C(N(C3=CC=C(SC)C=C3)C4=CC=C(SC)C=C4)C=C2)C(C5=CC=C(N(C6=CC=C(SC)C=C6)C7=CC=C(SC)C=C7)C=C5)=C(C)C(C8=CC=C(N(C9=CC=C(SC)C=C9)C%10=CC=C(SC)C=C%10)C=C8)=C1C%11=CC=C(N(C%12=CC=C(SC)C=C%12)C%13=CC=C(SC)C=C%13)C=C%11

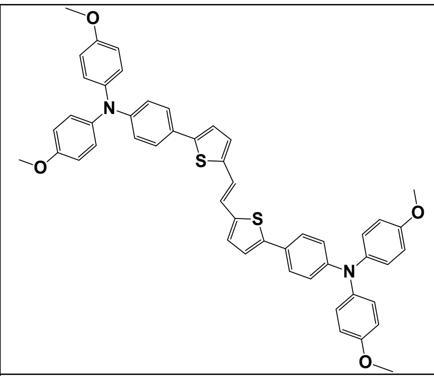
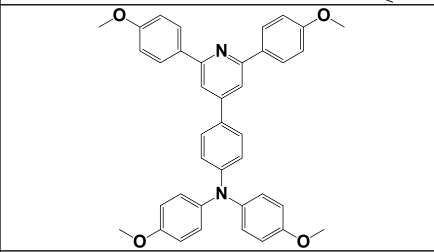
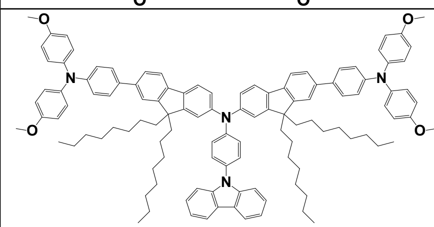
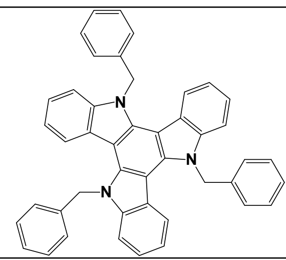
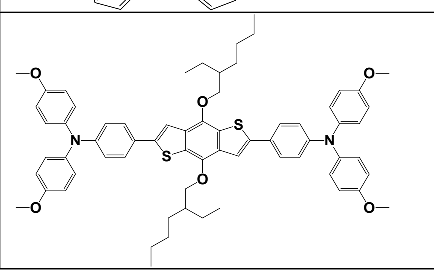
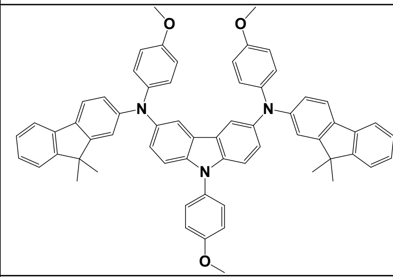
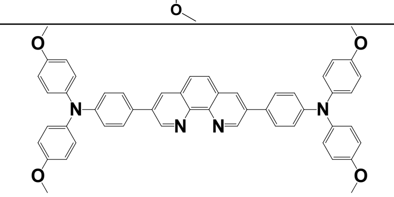
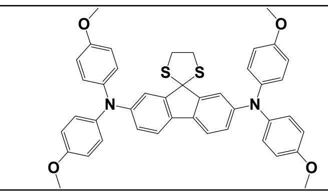
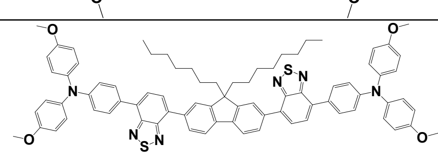
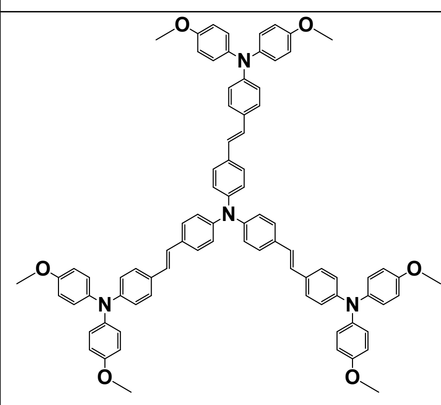
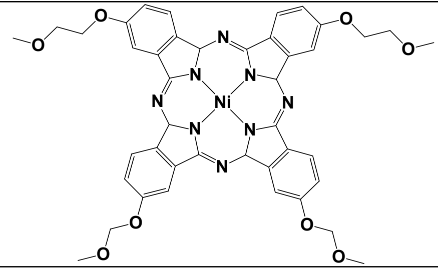
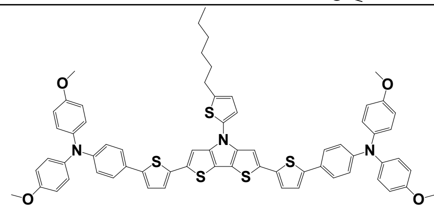
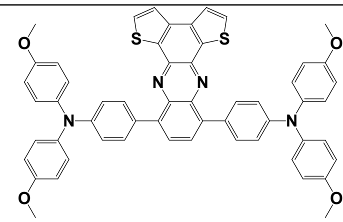
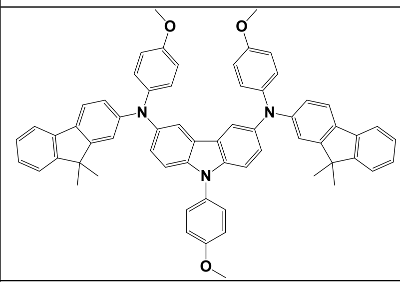
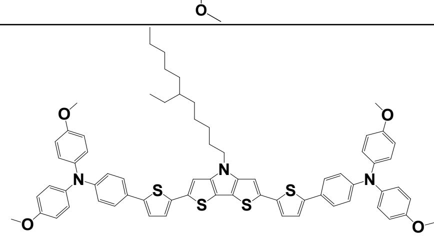
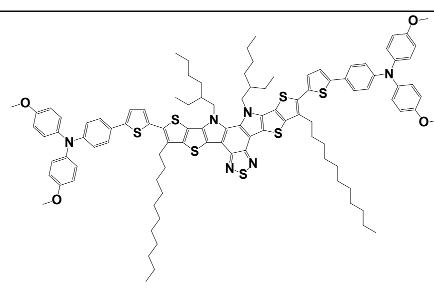
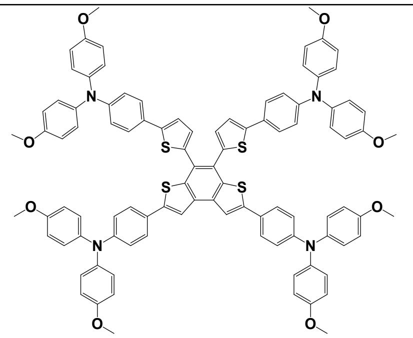
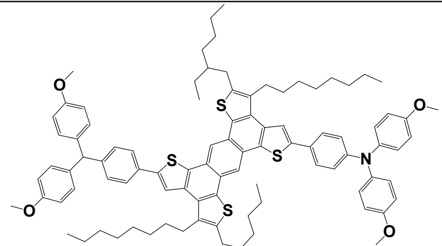
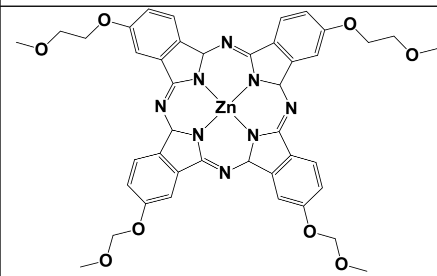
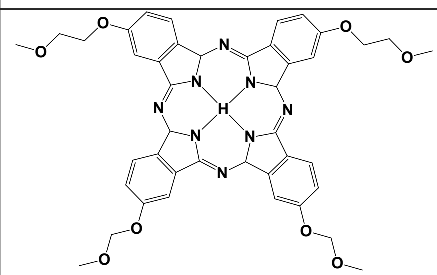
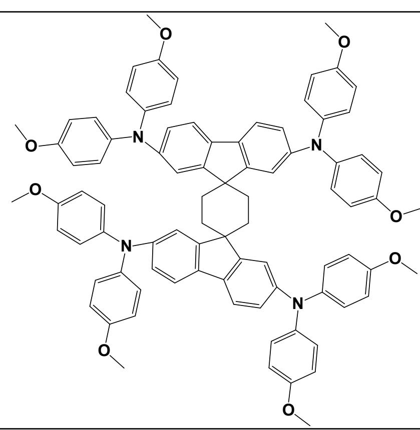
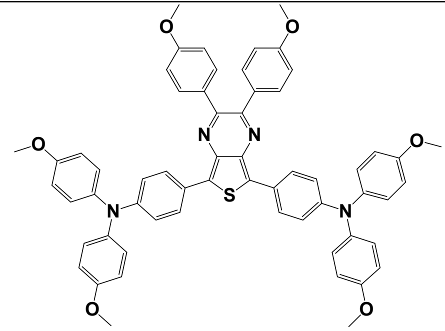
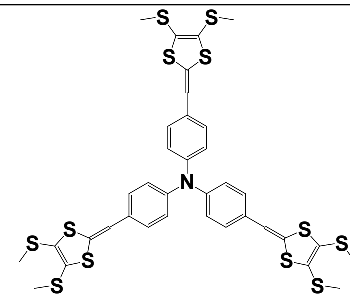
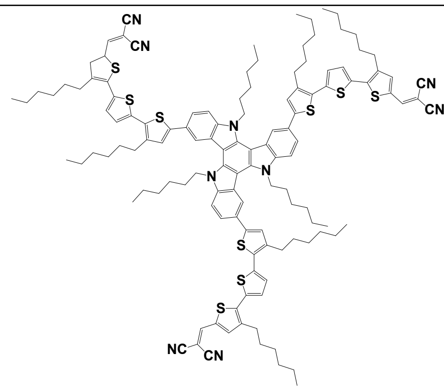
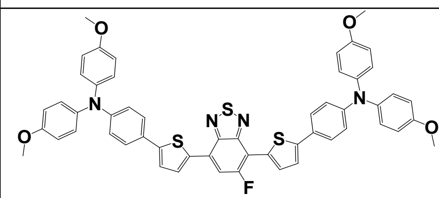
TPA-TVT-TPA	ITO/HTM/MAPbI_3/PCBM/BCP/Ag	1.07	21.49	0.71	16.32		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C(S4)=CC=C4/C=C/C5=CC=C(C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)S5
D104	ITO/HTM/MAPbI_3/$PC_{61}BM$/BCP/Ag	1.05	21.22	73.4	16.2		COC(C=C1)=CC=C1C2=CC(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)=CC(C6=CC=C(OC)C=C6)=N2
CzPAF-TPA	ITO/HTM/MAPbI_3/PCBM/ZnO/Ag	1.05	20	0.745	15.71		CCCCCCCCC(C1=C2C=CC(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)=C1)(CCCCCCCC)C6=C2C=CC(N(C7=CC=C(C(C=CC(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)=C%11)=C%11C%12(CCCCCCCC)CCCCCCCC)C%12=C7)C%13=CC=C(N%14C(C=CC=C%15)=C%15C%16=C%14C=CC=C%16)C=C%13)=C6
TBDI	ITO/MoO_3/HTM/MAPbI_3/IPH/PDINO/Ag	1.09	19.3	0.733	15.33		C1(N(CC2=CC=CC=C2)C3=C4C=CC=C3)=C4C(N(CC5=CC=CC=C5)C6=C7C=CC=C6)=C7C8=C1C9=C(C(=CC=C9)N8CC%10=CC=CC=C%10
H0	ITO/HTM/MAPbI_3/PC61BM/BCP/Ag	1.02	22.87	57.3	13.3		CCCCC(CC)COC1=C2C(C=C(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)S2)=C(OCC(CC)CCCC)C6=C1C=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)S6

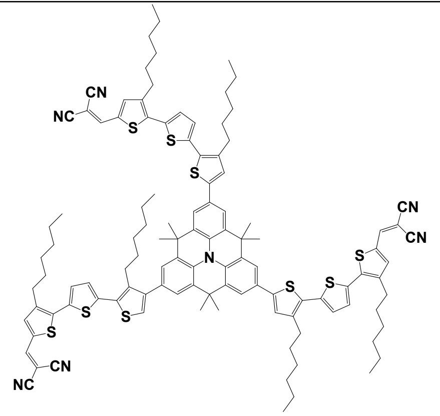
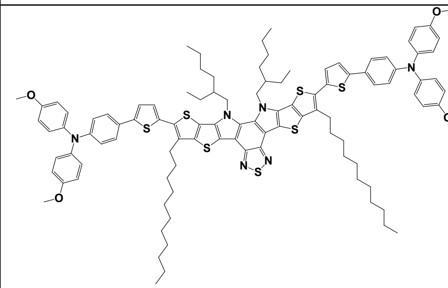
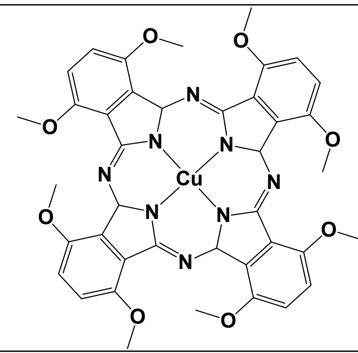
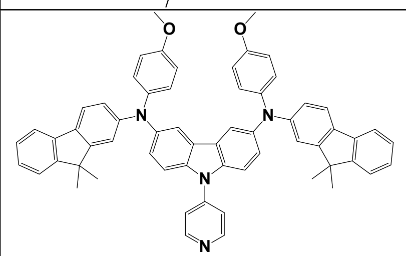
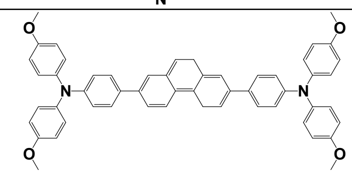
Table S2: Photovoltaic properties of dopant-free HTMs fabricated in mixed cation lead halide-based PSCs for conventional (n-i-p) and inverted (p-i-n) devices.

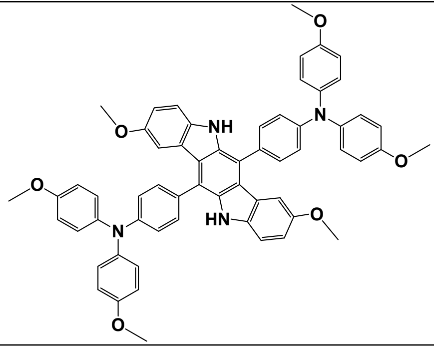
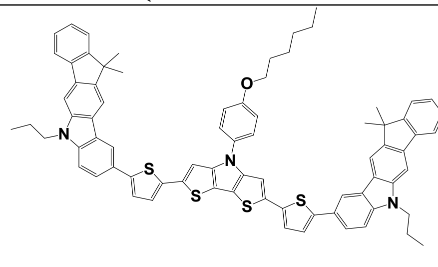
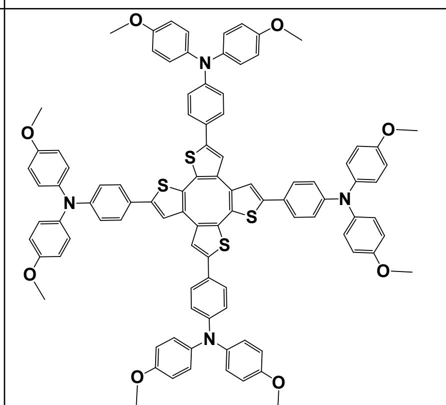
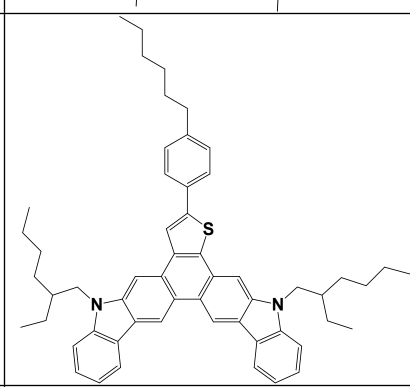
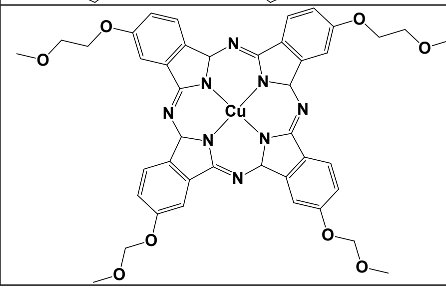
HTM	Device configuration	Voc [V]	Jsc [mAcm^{-2}]	FF [%]	PCE [%]	Structure	Smiles
Cz–As	FTO/ c-TiO_2/mpTiO_2/ PVK:CZ–Py/HTM/Au	1.15	25.20	81.2	23.5		CC(C1=C2C=CC=C1)(C)C3=C2C=CC(N(C4=CC=C(OC)C=C4)C5=CC6=C(C=C5)N(C7=CC=C(OC)C=C7)C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(C(C=CC=C%11)=C%11C%12(C)C)C%12=C%10)C=C86)=C3
YZ22	FTO/TiO_2/$Cs_{0.1}FA_{0.9}PbI_3$/HTM/Au	1.10	25.10	81.0	22.4		COC(C=C1)=CC=C1N(C(C=C2)=CC=C2C3=CC4=CC=C5C(N=CC(C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)=C5)=C4N=C3)C9=CC=C(OC)C=C9
SFDT –TMD	ITO/SnO_2/$Cs_xFA_{1\_x}PbI_3$ /HTM/MoO_3/ Ag	1.13	24.10	79.5	21.7		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3C45SCCS5)=CC=C3C6=C4C=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6
DTB-FL	ITO/SnO_2/$Cs_{0.05}FA_{0.95}PbI_3$/HTM/MoO_3/Ag	1.14	23.80	79.1	21.5		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC=C(C(C=C5)=CC(C6(CCCCCCCC)CCCCCCCC)=C5C(C=C7)=C6C=C7C8=CC=C(C9=NSN=C98)C%10=CC=C(N(C%11=CC=C(OC)C=C%11)C%12=CC=C(OC)C=C%12)C=C%10)C%13=NSN=C%134
MeOT TVT	FTO/c-TiO_2/m-TiO_2/$Cs_{0.05}(FA_{0.85}MA_{0.15})_{0.95}Pb(I_{0.85}Br_{0.15})_3$/ HTM/Au	1.11	23.89	80.3	21.3		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3/C=C/C(C=C4)=CC=C4N(C5=CC=C(/C=C/C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)C=C5)C9=CC=C(/C=C/C%10=CC=C(N(C%11=CC=C(OC)C=C%11)C%12=CC=C(OC)C=C%12)C=C%10)C=C9

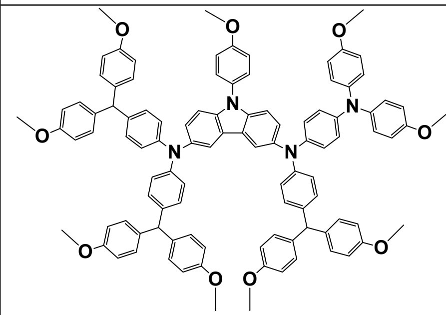
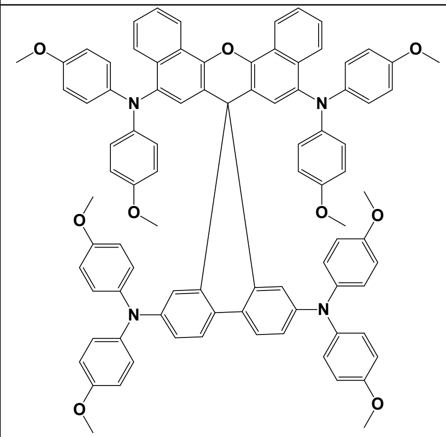
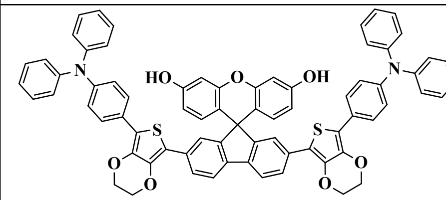
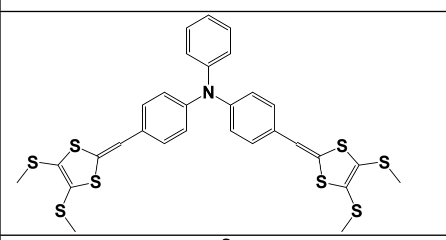
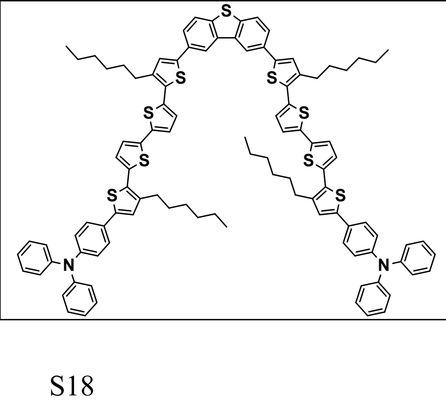
NiPc	FTO/ZnO/m-TiO_2/$Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$/HTM/Au	1.13	23.92	78.7	21.2		COCCOC(C=C1)=CC2=C1C3=NC4C(C=CC(OCCOC)=C5)=C5C6=NC(C7=C8C=C(OCOC)C=C7)N9C8=NC(C%10=C%11C=CC(OCOC)=C%10)N%12C%11=NC2N3[Ni]9%12N46
DTP-C6Th	FTO/SnO_2/C_{60}-SAM/$MA_{0.7}FA_{0.3}Pb(I_{0.925}Br_{0.075})_3$/PMMA/HTM/Au	1.15	22.76	0.79	21.04		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C(S4)=CC=C4C5=CC6=C(S5)C7=C(C=C(C8=CC=C(C9=CC=C(N(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)C=C9)S8)S7)N6C%12=CC=C(CCCCCC)S%12
TQ4	FTO/c-TiO_2/SnO_2/$Cs_{0.05}FA_{0.85}MA_{0.10}Pb(I_{0.97}Br_{0.03})_3$/HTM/Au)	1.12	23.71	79.0	21.0		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=C5C(N=C(C6=C7C=CS6)C(C8=C7C=CS8)=N5)=C(C9=CC=C(N(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)C=C9)C=C4
Cz–As	FTO/c-TiO_2/mpTiO_2/$FA_{0.9}$/$MA_{0.1}PbI_3$/HTM/Au	1.08	24.40	79.3	20.9		CC(C1=C2C=CC=C1)(C)C3=C2C=CC(N(C4=CC=C(OC)C=C4)C5=CC6=C(C=C5)N(C7=CC=C(OC)C=C7)C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(C(C=CC=C%11)=C%11C%12(C)C)C%12=C%10)C=C86)=C3
DTPC13-ThTPA	FTO/SnO_2/C_{60}-SAM/$MA_{0.7}FA_{0.3}PbI_{2.85}Br_{0.15}$/PMMA/HTM/Au	1.13	22.82	0.78	20.38		CCC(CCCCC)CCCCCN1C2=C(SC(C3=CC=C(C4=CC=C(N(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)C=C4)S3)=C2)C7=C1C=C(C8=CC=C(C9=CC=C(N(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)C=C9)S8)S7
Y-T	FTO/SnO_2/C_{60}-SAM/$MA_{0.7}FA_{0.3}PbI$/PEAI/HTM/Au	1.11	22.90	79.2	20.2		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC=C(S4)C(S5)=C(CCCCCCCCCCC)C6=C5C(N7CC(CCCC)CC)=C(S6)C8=C7C(N(CC(CCCC)CC)C9=C%10SC%11=C9SC(C%12=CC=C(C%13=CC=C(N(C%14=CC=C(OC)C=C%14)C%15=CC=C(OC)C=C%15)C=C%13)S%12)=C%11CCCCCCCCCCC)=C%10C%16=NSN=C%168

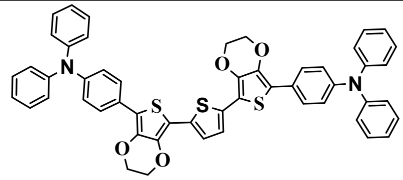
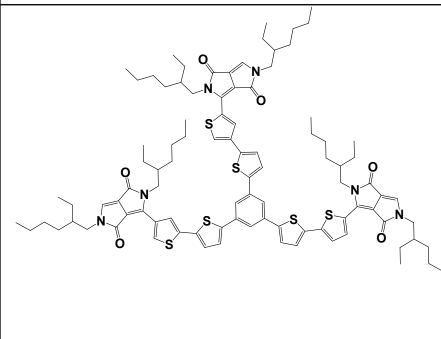
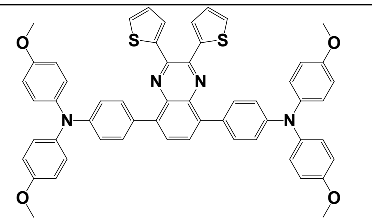
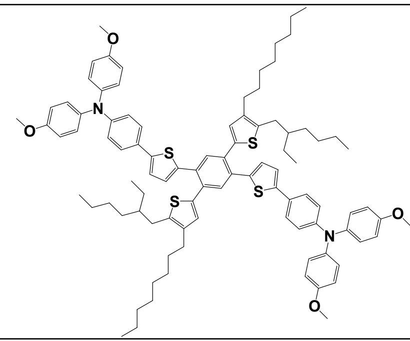
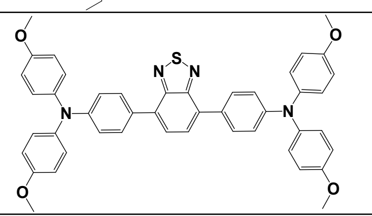
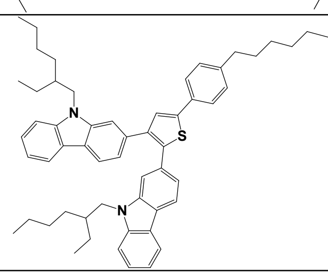
TTE-2	ITO/SnO_2/$(FAPbI_3)_{0.95}(MAPbBr_3)_{0.05}$/HTM/Au	1.11	23.26	0.77	20.04		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC=C(S4)C5=C(C6=CC=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)S6)C(SC(C%10=CC=C(N(C%11=CC=C(OC)C=C%11)C%12=CC=C(OC)C=C%12)C=C%10)=C%13)=C%13C%14=C5SC(C%15=CC=C(N(C%16=CC=C(OC)C=C%16)C%17=CC=C(OC)C=C%17)C=C%15)=C%14
ZT-H2	ITO/SnO_2/$MA_{1\_x}FA_xPbI_yCl_{3-y}$/HTM/$MoO_3$/Ag	1.11	24.15	73.4	19.6		CCCCCCCCC1=C(CC(CCCC)CC)SC2=C1C3=C(SC(C4=CC=C(C(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)C=C4)=C3)C7=CC(C8=C9C(CCCCCCCC)=C(CC(CCCC)CC)S8)=C(C%10=C9C=C(C%11=CC=C(N(C%12=CC=C(OC)C=C%12)C%13=CC=C(OC)C=C%13)C=C%11)S%10)C=C72
CuPc	FTO/ZnO/m-TiO_2/$Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$/HTM/Au	1.10	23.96	74.1	19.6		COCCOC(C=C1)=CC2=C1C3=NC4C(C=CC(OCCOC)=C5)=C5C6=NC(C7=C8C=C(OCOC)C=C7)N9C8=NC(C%10=C%11C=CC(OCOC)=C%10)N%12C%11=NC2N3[Zn]9%12N46
H2Pc	FTO/ZnO/m-TiO_2/$Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$/HTM/Au	1.11	23.85	74.4	19.6		COCCOC(C=C1)=CC2=C1C3=NC4C(C=CC(OCCOC)=C5)=C5C6=NC(C7=C8C=C(OCOC)C=C7)N9C8=NC(C%10=C%11C=CC(OCOC)=C%10)N%12C%11=NC2N3[H]9%12N46
WH-1	FTO/c-TiO_2/m-TiO_2/$CsMAFAPbIxBr_{3\_x}$/HTM/Au	1.08	23.37	77.5	19.5		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC4=C3C5=CC=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5C4(CC8)CCC8(C9=C%10C=CC(N(C%11=CC=C(OC)C=C%11)C%12=CC=C(OC)C=C%12)=C9)C%13=C%10C=CC(N(C%14=CC=C(OC)C=C%14)C%15=CC=C(OC)C=C%15)=C%13

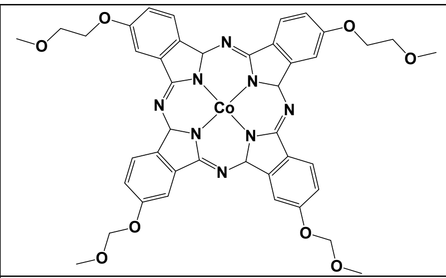
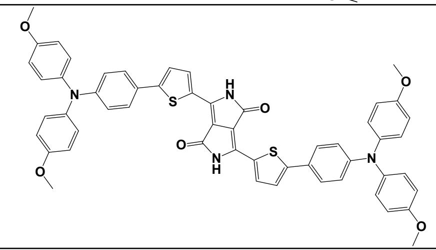
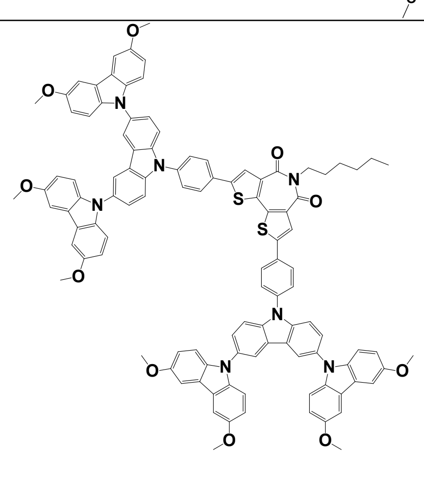
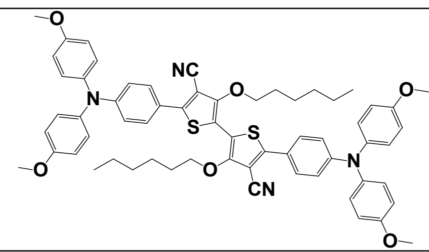
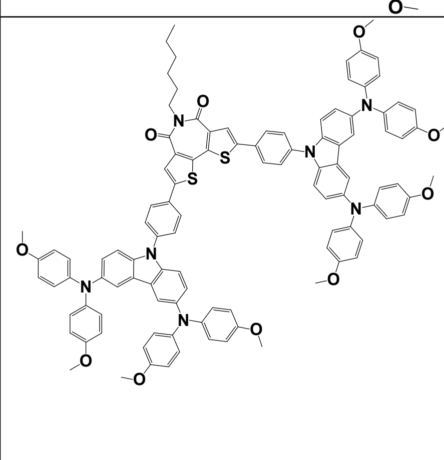
YN2	FTO/TiO_2/meso-TiO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTM/Au	1.11	22.87	0.75	19.27		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(C4=C(N=C(C5=CC=C(OC)C=C5)C(C6=CC=C(OC)C=C6)=N7)C7=C(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)S4)C=C3
WH-3	FTO/c-TiO_2/m-TiO_2/$Cs_{0.05}(FA_{0.85}MA_{0.15})_{0.95}Pb(I_{0.85}Br_{0.15})_3$/HTM/Au	1.07	23.05	77.9	19.2		CSC1=C(SC)SC(S1)=CC(C=C2)=CC=C2N(C3=CC=C(C=C4SC(SC)=C(SC)S4)C=C3)C5=CC=C(C=C6SC(SC)=C(SC)S6)C=C5
KR321	FTO/TiO_2/meso-TiO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTM/Au	1.13	21.7	0.78	19.03		CCCCCCC1=C(C2=CC=C(C3=C(CCCCCC)CC(/C=C(C#N)/C#N)S3)S2)SC(C4=CC(C(C(N(CCCCCC)C5=C6C=C(C7=CC(CCCCCC)=C(C8=CC=C(C9=C(CCCCCC)C=C(/C=C(C#N)/C#N)S9)S8)S7)C=C5)=C6C%10=C%11C%12=C(C=CC(C%13=CC(CCCCCC)=C(C%14=CC=C(C%15=C(CCCCCC)C=C(/C=C(C#N)\C#N)S%15)S%14)S%13)=C%12)N%10CCCCCC)=C%11N%16CCCCCC)=C%16C=C4)=C1
tpa-t-FBTD	FTO/SnO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTM/Au	1.08	22.40	78.1	18.9		FC1=C(C2=CC=C(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)S2)C6=NSN=C6C(C(S7)=CC=C7C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)=C1

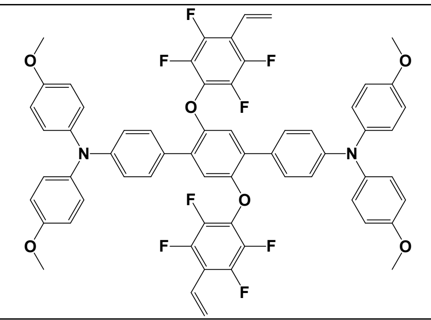
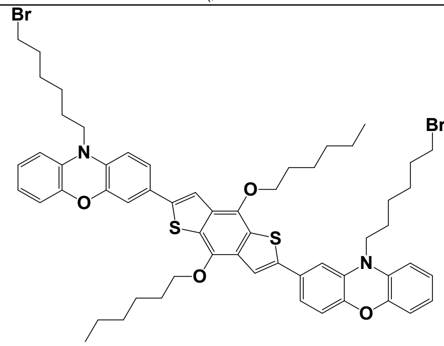
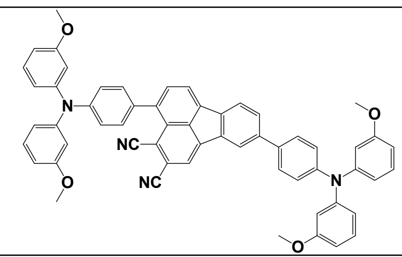
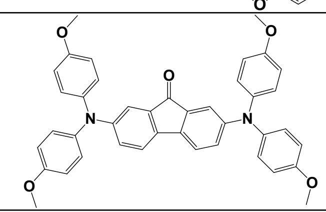
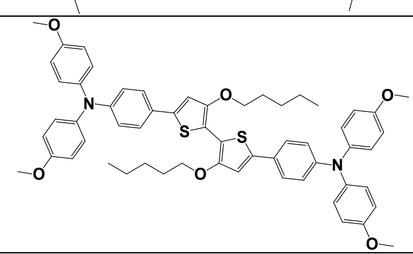
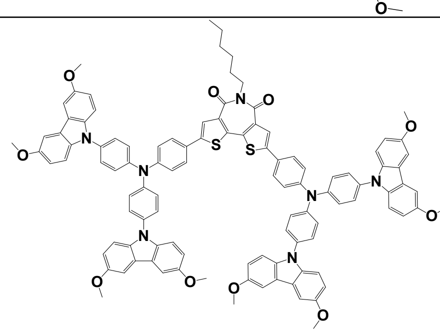
FA-CN	FTO/TiO_2/meso-TiO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTM/Au	1.13	21.71	0.77	18.9		CC(C1=C2C(C(C)(C)C3=CC(C4=CC(CCCCCC)=C(C5=CC=C(C6=C(CCCCCC)C=C(/C=C(C#N)/C#N)S6)S5)S4)=C7)=CC(C8=CSC(C9=CC=C(C%10=C(CCCCCC)C=C(/C=C(C#N)/C#N)S%10)S9)=C8CCCCCC)=C1)(C)C%11=C(N2C3=C7C%12(C)C)C%12=CC(C%13=CC(CCCCCC)=C(C%14=CC=C(C%15=C(CCCCCC)C=C(/C=C(C#N)\C#N)S%15)S%14)S%13)=C%11
Y6-T	FTO/SnO_2/C_{60}-SAM/$MA_{0.7}FA_{0.3}PbI$/PEAI/HTM/Au	1.10	22.90	74.1	18.8		CCCCCCCCCCCC1=C(C2=CC=C(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)S2)SC6=C1SC7=C6N(CC(CCCC)CC)C8=C7C9=NSN=C9C%10=C8N(CC(CCCC)CC)C%11=C%10SC%12=C%11SC(C%13=CC=C(C%14=CC=C(N(C%15=CC=C(OC)C=C%15)C%16=CC=C(OC)C=C%16)C=C%14)S%13)=C%12CCCCCCCCCCC
CuPc-(OMe)$_8$	FTO/SnO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTM/Au	1.05	22.10	79.0	18.3		COC1=CC=C(OC)C2=C1C3N4C2=NC(N5[Cu]674)C(C(OC)=CC=C8OC)=C8C5=NC(C9=C%10C(OC)=CC=C9OC)N6C%10=NC(C%11=C%12C(OC)=CC=C%11OC)N7C%12=N3
Cz–Py	FTO/ c-TiO_2/mpTiO_2/$FA_{0.9}/MA_{0.1}PbI_3$/HTM/Au	1.13	21.90	73.7	18.2		CC(C1=C2C=CC=C1)(C)C3=C2C=CC(N(C4=CC=C(OC)C=C4)C5=CC6=C(C=C5)N(C7=CC=NC=C7)C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(C(C=CC=C%11)=C%11C%12(C)C)C%12=C%10)C=C86)=C3
YZ18	FTO/TiO_2/$Cs_{0.1}FA_{0.9}PbI_3$/HTM/Au	1.03	24.10	73.0	18.1		COC(C=C1)=CC=C1N(C(C=C2)=CC=C2C3=CCC4=C5C=CC(C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)=CC5=CCC4=C3)C9=CC=C(OC)C=C9

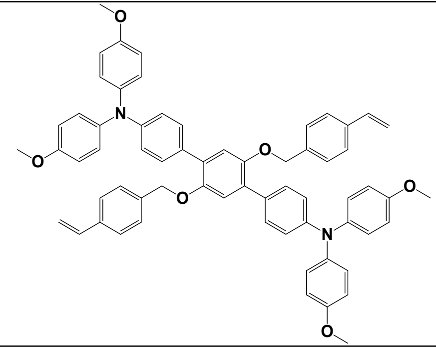
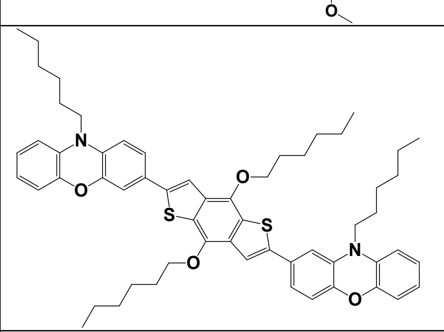
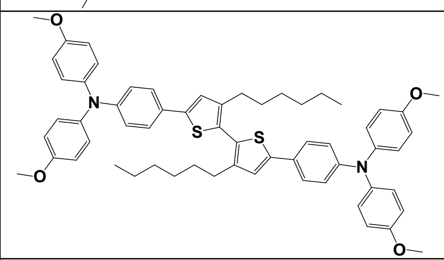
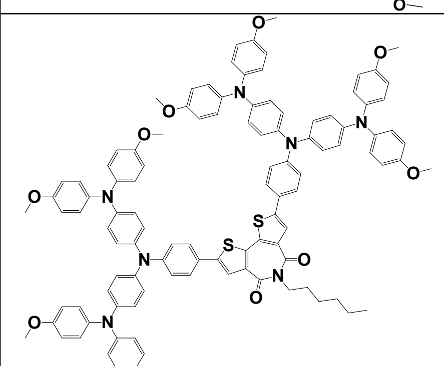
C202	FTO/TiO_2/meso-TiO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTM/Au	1.05	23	0.73	17.7		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(C4=C(NC5=C6C=C(OC)C=C5)C6=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)C%10=C4C%11=C(C=CC(OC)=C%11)N%10)C=C3
M129	ITO/SnO_2/PCBM/$Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$/HTM/Au	1.08	22.5	0.72	17.5		[c3H7]N(C1=CC(C(C=CC=C2)=C2C3(C)C)=C3C=C14)C(C4=C5)=CC=C5C(S6)=CC=C6C7=CC8=C(S7)C9=C(C=C(C%10=CC=C(C%11=CC%12=C(N(C%13=C%12C=C(C(C)(C)C%14=C%15C=CC=C%14)C%15=C%13)CCC)C=C%11)S%10)S9)N8C%16=CC=C(OCCCCCC)C=C%16
α, β-COTh-Ph-OMeTAD	FTO/TiO_2/meso-TiO_2/$(CsPbI_3)_{0.05}(FAPbI_3)_{0.79}(MAPbBr_3)_{0.16}$/HTM/Au	1.05	21.51	0.76	17.2		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC5=C(C6=C(C=C(C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)S6)C%10=C(C%11=C5C=C(C%12=CC=C(N(C%13=CC=C(OC)C=C%13)C%14=CC=C(OC)C=C%14)C=C%12)S%11)SC(C%15=CC=C(N(C%16=CC=C(OC)C=C%16)C%17=CC=C(OC)C=C%17)C=C%15)=C%10)S4
C302	FTO/c-TiO_2/m-TiO2/$(FAPbI_3)_{0.85}(MAPbBr_{0.15})$/HTM/Au	1.01	23.30	69.5	16.4		CCC(CCCC)CN1C2=CC(C3=C(C4=C5C=C(C(C=CC=C6)=C6N7CC(CC)CCCC)C7=C4)SC(C8=CC=C(CCCCCC)C=C8)=C3)=C5C=C2C9=C1C=CC=C9
ZnPc	FTO/ZnO/m-TiO_2/$Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$/HTM/Au	1.06	22.91	67.7	16.4		COCCOC(C=C1)=CC2=C1C3=NC4C(C=CC(OCCOC)=C5)=C5C6=NC(C7=C8C=C(OCOC)C=C7)N9C8=NC(C%10=C%11C=CC(OCOC)=C%10)N%12C%11=NC2N3[Cu]9%12N46

PhCz-4MeOTPA	FTO/TiO_2/meso-TiO_2/$Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$/HTM/Au	1.08	21.52	0.69	16.0		COC(C=C1)=CC=C1C(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3N(C4=CC=C(C(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)C=C4)C7=CC(C8=CC(N(C9=CC=C(N(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)C=C9)C%12=CC=C(C(C%13=CC=C(OC)C=C%13)C%14=CC=C(OC)C=C%14)C=C%12)=CC=C8N%15C%16=CC=C(OC)C=C%16)=C%15C=C7
X62	FTO/TiO_2/Mixed-PVK/HTM/Au/meso-TiO_2	1.01	22.4	0.70	15.9		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C34)=CC=C3C5=CC=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5C84C9=C(C(C=CC=C%10)=C%10C(N(C%11=CC=C(OC)C=C%11)C%12=CC=C(OC)C=C%12)=C9)OC%13=C8C=C(N(C%14=CC=C(OC)C=C%14)C%15=CC=C(OC)C=C%15)C%16=C%13C=CC=C%16
Spiro-IA	FTO/cl-TiO_2/mp-TiO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTMs/Au/Ag	1.04	22.14	0.67	15.7		OC1=CC(OC(C=C(O)C=C2)=C2C34C5=C(C6=C4C=C(C7=C8OCCOC8=C(C(C=C9)=CC=C9N(C%10=CC=CC=C%10)C%11=CC=CC=C%11)S7)C=C6)C=CC(C%12=C%13OCCOC%13=C(C(C=C%14)=CC=C%14N(C%15=CC=CC=C%15)C%16=CC=CC=C%16)S%12)=C5)=C3C=C1
WH-2	FTO/c-TiO_2/m-TiO_2/$Cs_{0.05}(FA_{0.85}MA_{0.15})_{0.95}Pb(I_{0.85}Br_{0.15})_3$/HTM/Au	1.02	21.95	68.7	15.3		CSC1=C(SC)SC(S1)=CC(C=C2)=CC=C2N(C3=CC=C(C=C4SC(SC)=C(SC)S4)C=C3)C5=CC=CC=C5
DBT(QT-TPA)$_2$	FTO/cl-TiO_2/mp-TiO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTMs/Au/Ag	1.04	19.23	0.68	13.6		CCCCCCC1=C(SC(C2=CC3=C(C=C2)SC4=C3C=C(C5=CC(CCCCCC)=C(S5)C(S6)=CC=C6C(S7)=CC=C7C8=C(CCCCCC)C=C(S8)C(C=C9)=CC=C9N(C%10=CC=CC=C%10)C%11=CC=CC=C%11)C=C4)=C1)C(S%12)=CC=C%12C(S%13)=CC=C%13C%14=C(CCCCCC)C=C(S%14)C(C=C%15)=CC=C%15N(C%16=CC

							=CC=C%16)C%17=CC=C C=C%17
T(EDOT-TPA)$_2$	FTO/cl-TiO_2/mp-TiO_2/$(FAPbI_3)_{0.85}(MAPbBr_3)_{0.15}$/HTMs/Au/Ag	1.04	20.25	0.58	12.3		C1(N(C2=CC=CC=C2)C3=CC=C(C4=C5C(OCCO5)=C(C6=CC=C(C7=C8OCCOC8=C(C(C=C9)=CC=C9N(C%10=CC=CC=C%10)C%11=CC=CC=C%11)S7)S6)S4)C=C3)=CC=CC=C1
TB-DPP	ITO/SnO_2/$FA_{0.85}MA_{0.15}PbI_3$/HTMs/MoO_3/Ag	1.03	18.97	59.4	11.6		O=C(N1CC(CCCC)CC)C(C2=C1C3=CC=C(S3)C(S4)=CC=C4C5=CC(C6=CC=C(C7=CSC(C8=C9C(C(N8CC(CCCC)CC)=O)=CN(CC(CC)CCCC)C9=O)=C7)S6)=CC(C%10=CC=C(C%11=CC(C%12=C%13C(C(N%12CC(CC)CCCC)=O)=CN(CC(CC)CCCC)C%13=O)=CS%11)S%10)=C5)=CN(CC(CCCC)CC)C2=O
TQ3	FTO/c-TiO_2/SnO_2/$Cs_{0.05}FA_{0.85}MA_{0.10}Pb(I_{0.97}Br_{0.03})_3$/HTM/Au)	0.95	20.90	45.0	10.8		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=C5C(N=C(C6=CC=CS6)C(C7=CC=CS7)=N5)=C(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)C=C4
ZT-H1	ITO/SnO_2/$MA_{1\_x}FA_xPbI_yCl_{3-y}$/HTM/$MoO_3$/Ag	1.00	21.21	47.6	10.0		CCC(CCCC)CC(S1)=C(CCCCCCCC)C=C1C2=CC(C3=CC=C(C4=CC=C(N(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)C=C4)S3)=C(C7=CC(CCCCCCCC)=C(CC(CCCC)CC)S7)C=C2C8=CC=C(C9=CC=C(C(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)C=C9)S8
DT-BT	ITO/SnO_2/$Cs_{0.05}FA_{0.95}PbI_3$/HTM/MoO_3/Ag	0.83	16.80	52.2	7.30		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C(C=C3)=CC=C3C4=CC=C(C5=CC=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5)C8=NSN=C84
C301	FTO/c-TiO_2/m-TiO_2/$(FAPbI_3)_{0.85}(MAPbBr_{0.15})$/HTM/Au	0.73	19.60	40.6	5.8		CCC(CCCC)CN1C2=CC(C3=C(C4=CC=C(C(C=CC=C5)=C5N6CC(CC)CCCC)C6=C4)SC(C7=CC=C(CCCCCC)C=C7)=C3)=CC=C2C8=C1C=CC=C8

CoPc	FTO/ZnO/m-TiO_2/$Cs_{0.05}(MA_{0.17}FA_{0.83})_{0.95}Pb(I_{0.83}Br_{0.17})_3$/HTM/Au	0.96	11.03	51.3	5.4		COCCOC(C=C1)=CC2=C1C3=NC4C(C=CC(OCCOC)=C5)=C5C6=NC(C7=C8C=C(OCOC)C=C7)N9C8=NC(C%10=C%11C=CC(OCOC)=C%10)N%12C%11=NC2N3[Co]9%12N46
TPADPP	ITO/HTM/$FA_{0.8}Cs_{0.2}PbI_{2.96}Br_{0.04}$/$C_{60}$/BCP/Ag	1.12	23.72	83.0	21.6		O=C(N1)C(C2=C1C3=CC=C(S3)C4=CC=C(N(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)C=C4)=C(C7=CC=C(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)S7)NC2=O
MCz–Cz–BTI	ITO/HTM/CsMAFAPbIxBr$_{3_x}$/C_{60}/BCP/Ag	1.10	23.24	83.5	21.3		O=C(C1=C(C2=C3C=C(C4=CC=C(N5C6=CC=C(N7C8=CC=C(OC)C=C8C9=C7C=CC(OC)=C9)C=C6C%10=C5C=CC(N(C%11=CC=C(OC)C=C%11%12)C%13=C%12C=C(OC)C=C%13)=C%10)C=C4)S2)SC(C%14=CC=C(N%15C%16=CC=C(N%17C%18=CC=C(OC)C=C%18C%19=C%17C=CC(OC)=C%19)C=C%16C%20=C%15C=CC(N(C%21=CC=C(OC)C=C%21%22)C%23=C%22C=C(OC)C=C%23)=C%20)C=C%14)=C1)N(CCCCCC)C3=O
BTORCNA	ITO/HTM/$(FA_{0.17}MA_{0.94}PbI_{3.11})_{0.95}(PbCl_2)$/$C_{60}$/BCP/Ag	1.10	22.84	84.0	21.1		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(C4=C(C#N)C(OCCCCCC)=C(C5=C(OCCCCCC)C(C#N)=C(C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)S5)S4)C=C3
MPA–Cz–BTI	ITO/HTM/CsMAFAPbIxBr$_{3_x}$/C_{60}/BCP/Ag	1.07	22.84	85.2	20.8		O=C(C1=C(C2=C3C=C(C4=CC=C(N5C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6C9=C5C=CC(N(C%10=CC=C(OC)C=C%10)C%11=CC=C(OC)C=C%11)=C9)C=C4)S2)SC(C%12=CC=C(N%13C%14=CC=C(N(C%15=CC=C(OC)C=C%15)C%16=CC=C(OC)C=C%16)C=C%14C%17=C%13C=CC(N(C%18=CC=C(OC)C=C%18)C%19=CC=C(OC)C=C%19)=C%17)C=C%12)=C1)N(CCCCCC)C3=O

HTM-F	ITO/HTM/$(FAPbI_3)_{1-x}(MAPbBr_3)$/$C_{60}$/BCP/Ag	1.09	23.03	82.0	20.5		C=CC1=C(F)C(F)=C(OC2=CC(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)=C(OC6=C(F)C(F)=C(C=C)C(F)=C6F)C=C2C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7)C(F)=C1F
N01	ITO/HTM/$Cs_{0.05}(FA_{0.95}MA_{0.05})_{0.95}Pb(I_{0.95}Br_{0.05})_3$/$C_{60}$/BCP/Ag	1.08	23.65	80.1	20.4		CCCCCCOC1=C2C(C=C(C3=CC(OC(C=CC=C4)=C4N5CCCCCCBr)=C5C=C3)S2)=C(OCCCCCC)C6=C1C=C(C7=CC=C(OC(C=CC=C8)=C8N9CCCCCCBr)C9=C7)S6
BTF6	ITO/HTM/$(FA_{0.92}MA_{0.08})Cs_{0.1}Pb(I_{0.92}Br_{0.08})_3$/$C_{60}$/BCP/Ag	1.13	22.23	81.0	20.3		N#CC(C=C12)=C(C#N)C3=C1C(C4=C2C=C(C5=CC=C(N(C6=CC=CC(OC)=C6)C7=CC(OC)=CC=C7)C=C5)C=C4)=CC=C3C8=CC=C(N(C9=CC=CC(OC)=C9)C%10=CC(OC)=CC=C%10)C=C8
TPA-FO	ITO/HTM/$(FA_{0.17}MA_{0.94}PbI_{3.11})_{0.95}(PbCl_2)_{0.05}$/LiF/$C_{60}$/BCP/Ag	1.09	22.76	81.8	20.2		O=C1C2=C(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C31)C=CC(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)=C2
BTORA	ITO/HTM/$(FA_{0.17}MA_{0.94}PbI_{3.11})_{0.95}(PbCl_2)$/$C_{60}$/BCP/Ag	1.09	22.10	83.4	20.2		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(C4=CC(OCCCCC)=C(C5=C(OCCCCC)C=C(C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)S5)S4)C=C3
MCz–PA–BTI	ITO/HTM/CsMAFAPbIxBr3_x/C_{60}/BCP/Ag	1.08	22.66	82.1	20.0		O=C(C1=C(C2=C3C=C(C4=CC=C(N(C5=CC=C(N(C6=CC=C(OC)C=C67)C8=C7C=C(OC)C=C8)C=C5)C9=CC=C(N%10C%11=CC=C(OC)C=C%11C%12=C%10C=CC(OC)=C%12)C=C9)C=C4)S2)SC(C%13=CC=C(N(C%14=CC=C(N(C%15=CC=C(OC)C=C%15%16)C%17=C%16C=C(OC)C=C%17)C=C%14)C%18=CC=C

							(N%19C%20=CC=C(OC)C=C%20C%21=C%19C=CC(OC)=C%21)C=C%18)C=C%13)=C1)N(CCCCCC)C3=O
HTM-H	ITO/HTM/$(FAPbI_3)_{1-x}$(MAPbBr3)/C60/BCP/Ag	1.05	22.70	80.0	19.0		C=CC(C=C1)=CC=C1COC2=CC(C3=CC=C(N(C4=CC=C(OC)C=C4)C5=CC=C(OC)C=C5)C=C3)=C(OCC6=CC=C(C=C)C=C6)C=C2C7=CC=C(N(C8=CC=C(OC)C=C8)C9=CC=C(OC)C=C9)C=C7
N02	ITO/HTM/$Cs_{0.05}(FA_{0.95}MA_{0.05})_{0.95}Pb(I_{0.95}Br_{0.05})_3/C_{60}$/BCP/Ag	1.03	23.48	78.3	18.9		CCCCCCOC1=C2C(C=C(C3=CC(OC(C=CC=C4)=C4N5CCCCCC)=C5C=C3)S2)=C(OCCCCCC)C6=C1C=C(C7=CC=C(OC(C=CC=C8)=C8N9CCCCCC)C9=C7)S6
BTRA	ITO/HTM/$(FA_{0.17}MA_{0.94}PbI_{3.11})_{0.95}(PbCl_2)/C_{60}$/BCP/Ag	1.06	21.64	80.1	18.4		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(C4=CC(CCCCCC)=C(C5=C(CCCCCC)C=C(C6=CC=C(N(C7=CC=C(OC)C=C7)C8=CC=C(OC)C=C8)C=C6)S5)S4)C=C3
MPA-PA-BTI	ITO/HTM/CsMAFAPbIxBr$_{3_x}$/C_{60}/BCP/Ag	0.99	22.15	79.4	17.4		O=C(C1=C(C2=C3C=C(C4=CC=C(N(C5=CC=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5)C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)C=C4)S2)SC(C%11=CC=C(N(C%12=CC=C(N(C%13=CC=C(OC)C=C%13)C%14=CC=C(OC)C=C%14)C=C%12)C%15=CC=C(N(C%16=CC=C(OC)C=C%16)C%17=CC=C(OC)C=C%17)C=C%15)C=C%11)=C1)N(CCCCCC)C3=O

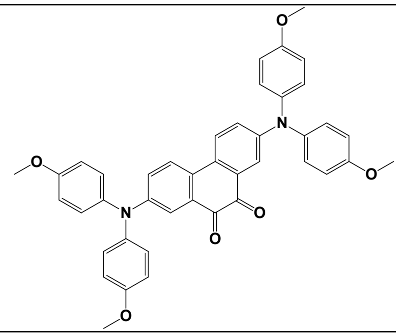
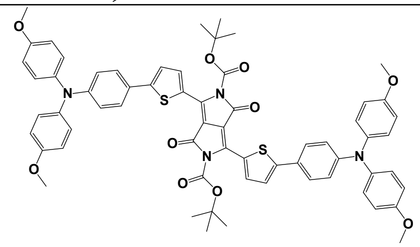
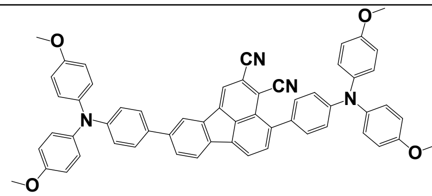
TPA-PDO	ITO/HTM/($FA_{0.17}MA_{0.94}PbI_{3.11})_{0.95}(PbCl_2)_{0.05}$/LiF/$C_{60}$/BCP/Ag	1.03	20.44	80.9	17.0		O=C(C1=O)C2=C(C=CC(N(C3=CC=C(OC)C=C3)C4=CC=C(OC)C=C4)=C2)C5=C1C=C(N(C6=CC=C(OC)C=C6)C7=CC=C(OC)C=C7)C=C5
TPAD PP-Boc	ITO/HTM/$FA_{0.8}Cs_{0.2}PbI_{2.96}Br_{0.04}$/$C_{60}$/BCP/Ag	1.02	22.22	72.0	16.3		O=C(N1C(OC(C)(C)C)=O)C(C2=C1C3=CC=C(S3)C4=CC=C(N(C5=CC=C(OC)C=C5)C6=CC=C(OC)C=C6)C=C4)=C(C7=CC=C(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)S7)N(C(OC(C)(C)C)=O)C2=O
BTF5	ITO/HTM/($FA_{0.92}MA_{0.08}$)$Cs_{0.1}Pb(I_{0.92}Br_{0.08})_3$/$C_{60}$/BCP/Ag	0.80	21.31	67.0	11.4		COC(C=C1)=CC=C1N(C2=CC=C(OC)C=C2)C3=CC=C(C4=CC=C5C6=C4C(C#N)=C(C#N)C=C6C7=C5C=CC(C8=CC=C(N(C9=CC=C(OC)C=C9)C%10=CC=C(OC)C=C%10)C=C8)=C7)C=C3

Table (S3): Experimental and predicted PCE, V_{OC}, and J_{SC} values for the test and train sets for dopant free HTMs when used in **PSCs** devices utilizing 1D, and 2D descriptors.

HTM	PCE				V_{OC}				J_{SC}			
	Set	Y (Obs)	Y (Pred)	Error	Set	Y (Obs)	Y (Pred)	Error	Set	Y (Obs)	Y (Pred)	Error
TAT-2T-CAN	train	20.1	17.8324	-2.2676	train	1.13	1.1006	-0.0294	test	23.1	23.0397	-0.0603
C-CPDT	test	19.6	16.9849	-2.6151	train	1.14	1.0166	-0.1234	train	23.27	22.6329	-0.6371
FBA3	train	19.27	16.1334	-3.1366	train	1.09	1.1156	0.0256	train	22.12	21.0126	-1.1074
FBA2	test	18.7	17.0126	-1.6874	train	1.06	1.0259	-0.0341	train	22.32	21.8086	-0.5114
CJ-01	train	18.56	18.1964	-0.3636	train	1.113	1.0477	-0.0653	train	22.32	22.3518	0.0318
TPA-BPFN-TPA	train	18.4	19.3958	0.9959	train	1.04	1.0272	-0.0128	train	22.7	22.4605	-0.2395
ACE-QA-ACE	train	18.2	19.4204	1.2204	train	1.06	1.0468	-0.0132	train	22.41	22.5908	0.1808
PCA-1	train	18.17	18.0004	-0.1697	test	1.062	1.0517	-0.0103	test	22.3	22.5158	0.2158
IDF-SFXPh	test	17.6	18.9861	1.3861	test	1.05	1.0678	0.0178	test	21.5	21.9417	0.4417
BTDTP	train	17.6	17.742	0.142	train	0.97	1.0146	0.0446	train	25.73	24.7221	-1.0079
TPA-3T-DCV	train	17.6	17.7235	0.1235	test	1.08	1.0946	0.0146	test	23	21.7325	-1.2675
TAT-2T-DCV	train	17.6	18.0348	0.4348	train	1.08	1.1094	0.0294	train	23	22.7035	-0.2965
TPA-ANT-TPA	train	17.5	17.8301	0.3301	test	1.03	1.0317	0.0017	train	21.07	21.7921	0.7221
BTPA-TCNE	train	16.94	18.8084	1.8684	test	1.04	1.0468	0.0068	train	20.84	20.8297	-0.0103
BTBDT	train	16.9	17.2279	0.3279	train	0.95	0.9917	0.0417	test	24.68	24.3215	-

												0.3585
FBA1	test	16.8	16.7927	-0.0073	train	1.05	0.9845	-0.0655	train	21.57	22.025	0.455
Z1011	train	16.3	16.9216	0.6216	train	1.096	1.0742	-0.0218	test	20.52	21.2274	0.7074
Z34	train	16.1	18.4876	2.3876	train	1.055	1.0867	0.0317	train	21.245	21.8401	0.5951
CQ2	train	15.2	17.05	1.85	train	1.02	1.0087	-0.0113	train	20.57	22.3313	1.7613
DTBT	train	11.6	16.1696	4.5696	train	0.93	0.9959	0.0659	test	22.2	22.6803	0.4803
DTBS	train	15	14.4899	-0.5101	train	0.96	0.9087	-0.0513	train	22.78	22.4247	-0.3553
DOR3T-TBDT	train	14.9	14.2318	-0.6682	train	0.97	0.9899	0.0199	train	20.7	21.1596	0.4596
X25	train	14.4	18.1915	3.7915	train	1.01	1.0431	0.0331	train	19.64	22.2926	2.6526
HTM1	train	13.4	17.4857	4.0857	train	0.971	1.0416	0.0706	train	19.3	21.4981	2.1981
DTBF	test	13.3	15.8713	2.5713	test	0.95	0.994	0.044	train	22.48	22.5984	0.1184
T-CPDT	train	11.4	16.5162	5.1162	train	0.88	0.9588	0.0788	train	21.37	22.0527	0.6827
DFBT-MTP	test	21.2	20.8406	-0.3594	test	1.16	1.1466	-0.0134	train	22.15	22.542	0.392
MPA-BTTI	train	21.17	19.9824	-1.1876	train	1.12	1.1037	-0.0163	train	23.23	23.3242	0.0942
DBTMT	test	21.1	21.0342	-0.0659	train	1.12	1.1301	0.0101	train	22.7	22.978	0.278
TPE-S	train	21	20.0462	-0.9538	train	1.13	1.0958	-0.0341	train	23.3	22.338	-0.962
DFH	train	20.6	20.1701	-0.4299	train	1.09	1.0878	-0.0022	test	22.7	22.8006	0.1006
DBFMT	test	20.5	20.7966	0.2966	train	1.07	1.0948	0.0248	test	23.7	22.9038	-0.7962
DPh-DNTT	train	20.1	16.97	-3.1301	train	1.1	1.1147	0.0147	train	22.56	21.7938	-0.7662
BT-MTP	train	20.1	21.1694	1.0694	train	1.1	1.1357	0.0357	train	23.01	23.0812	0.0712
YJ01	train	19.8	19.2874	-0.5126	train	1.08	1.0476	-0.0324	train	22.53	22.6554	0.1254
BDT-POZ	test	19.16	17.9635	-1.1965	train	1.04	1.0629	0.0229	train	22.56	22.8774	0.3174
FMT	train	19.06	19.3605	0.3005	test	1.07	1.0611	-0.0089	train	22.52	22.1675	-0.3525
TAPC	train	18.8	17.5165	-1.2835	train	1.04	0.9889	-0.0511	test	22.32	21.6082	-0.7118
XY1	train	18.78	17.0954	-1.6846	train	1.11	1.0373	-0.0727	train	22.21	21.8969	-0.3131
VB-MeO-FDPA	train	18.7	18.8392	0.1393	train	1.15	1.1056	-0.0444	train	20.89	21.5061	0.6161
Trux-OMeTAD	train	18.6	17.6879	-0.9121	train	1.02	0.9976	-0.0224	train	23.2	21.3787	-1.8213
H2	train	18.6	18.7745	0.1745	train	1.06	1.077	0.017	train	22.93	23.8954	0.9654
D106	train	18.2	18.6385	0.4385	train	1.05	1.0689	0.0189	train	22.32	22.5691	0.2491
m-MTDATA	train	18.12	17.7387	-0.3813	train	1.035	1.0131	-0.0219	test	22.5	21.3542	-1.1458
TPAC3M	train	17.54	17.4647	-0.0753	train	1	1.0061	0.0061	train	22.79	22.0671	-0.7229
YJ02	train	17.5	18.8715	1.3715	train	1.04	1.0379	-0.0021	train	22.22	22.4353	0.2153
D105	train	17.4	17.2494	-0.1506	train	1.04	1.0295	-0.0105	test	21.96	22.1226	0.1626
TPA-2,7-FLTPA-TPA	train	17.1	16.888	-0.212	test	1.052	0.9958	-0.0562	train	20.82	20.9445	0.1245
TTA	test	16.7	17.4256	0.7256	test	1.04	1.0014	-0.0386	train	20.4	19.078	-1.322
TPP-SMeTAD	train	16.6	19.7769	3.1769	train	1.07	1.0719	0.0019	train	20.15	22.0702	1.9202

TPA-TVT-TPA	train	16.32	17.3436	1.0236	train	1.07	1.0574	-0.0126	train	21.49	22.5209	1.0309
D104	train	16.2	16.9034	0.7034	train	1.05	1.0552	0.0052	train	21.22	21.6551	0.4352
CzPAF-TPA	train	15.71	17.1064	1.3964	train	1.05	1.0052	-0.0448	train	20	21.4196	1.4196
TBDI	test	15.33	14.613	-0.717	test	1.09	1.0325	-0.0575	train	19.3	19.9255	0.6255
H0	train	13.3	15.7115	2.4115	train	1.02	1.0242	0.0042	test	22.87	22.4008	-0.4692
YZ22	train	22.4	18.5943	-3.8057	train	1.1	1.0287	-0.0713	train	25.1	22.9657	-2.1344
SFDT-TMD	train	21.7	19.82	-1.88	test	1.13	1.0821	-0.0479	train	24.1	22.8018	-1.2982
MeOTTVT	train	21.3	18.6516	-2.6484	test	1.11	1.082	-0.028	train	23.89	22.0943	-1.7957
DTP-C6Th	train	21.04	18.3689	-2.6711	train	1.15	1.135	-0.015	train	22.76	22.4859	-0.2741
TQ4	train	21	17.4246	-3.5754	test	1.12	1.0451	-0.0749	train	23.71	23.1179	-0.5921
Cz-As	train	20.9	20.2878	-0.6122	train	1.08	1.112	0.032	train	24.4	23.2912	-1.1088
DTPC13-ThTPA	train	20.38	16.1654	-4.2146	train	1.13	1.0811	-0.0489	test	22.82	22.4389	-0.3811
TTE-2	train	20.04	17.9211	-2.1189	train	1.11	1.08	-0.03	train	23.26	21.8766	-1.3834
ZT-H2	train	19.6	15.7288	-3.8712	train	1.11	1.0644	-0.0456	train	24.15	21.977	-2.173
CuPc	train	19.6	18.8228	-0.7772	test	1.1	1.0203	-0.0797	test	23.96	21.7782	-2.1818
H2Pc	train	19.6	17.3385	-2.2615	train	1.11	1.1369	0.0269	train	23.85	22.7267	-1.1233
WH-1	train	19.5	19.5156	0.0156	train	1.08	1.0507	-0.0293	train	23.37	22.4898	-0.8802
YN2	train	19.27	17.3787	-1.8913	test	1.11	1.0719	-0.0381	train	22.87	22.5403	-0.3297
WH-3	train	19.2	16.6974	-2.5026	train	1.07	1.1018	0.0318	train	23.05	21.9045	-1.1455
tpa-t-FBTD	train	18.9	17.016	-1.884	train	1.08	1.0279	-0.0521	train	22.4	23.0922	0.6922
FA-CN	test	18.9	19.4296	0.5296	train	1.13	1.1312	0.0012	train	21.71	21.5253	-0.1847
Y6-T	train	18.8	15.4636	-3.3364	train	1.1	1.1081	0.0081	train	22.9	22.5659	-0.3341
Cz-Py	test	18.2	19.9092	1.7092	train	1.13	1.1251	-0.0049	train	21.9	23.2368	1.3368
YZ18	test	18.1	18.3234	0.2234	train	1.03	1.0335	0.0035	train	24.1	22.3597	-1.7403
C202	train	17.7	17.8157	0.1157	train	1.05	1.0337	-0.0163	train	23	22.8405	-0.1595
?, ?-COTh-Ph-OMeTAD	test	17.2	17.4095	0.2095	train	1.05	1.0422	-0.0078	train	21.51	21.4492	-0.0608
C302	train	16.4	12.376	-4.0239	train	1.01	0.8884	-0.1216	test	23.3	21.9045	-1.3955
PhCz-4MeOTPA	train	16	15.6281	-0.3719	test	1.08	1.0116	-0.0684	train	21.52	20.9704	-0.5496
X62	test	15.9	18.9536	3.0536	test	1.01	1.0691	0.0591	train	22.4	21.8445	-0.5555
Spiro-IA	train	15.7	14.5533	-1.1467	train	1.04	1.0398	-0.0002	train	22.14	21.3648	-0.7752
WH-2	train	15.3	15.1298	-0.1702	train	1.02	1.0444	0.0244	train	21.95	21.3362	-0.6138
2 DBT(QT-TPA)2	test	13.6	14.39	0.79	train	1.04	1.0324	-0.0076	train	19.23	20.5078	1.2778
T(EDOT-TPA)2	train	12.3	12.4157	0.1157	train	1.04	1.0613	0.0213	test	20.25	21.9342	1.6842
TQ3	train	10.8	16.4994	5.6994	test	0.95	1.0327	0.0827	test	20.9	22.5634	1.6634
ZT-H1	test	10	15.1471	5.1471	train	1	1.0386	0.0386	train	21.21	21.3449	0.1349

DT-BT	train	7.3	15.6685	8.3685	train	0.83	0.9445	0.1145	train	16.8	21.8383	5.0383
C301	train	5.8	11.6077	5.8077	train	0.73	0.8536	0.1236	test	19.6	21.7014	2.1014
TPADPP	train	21.6	19.2952	-2.3048	train	1.12	1.102	-0.018	train	23.72	23.3602	-0.3598
MCz-cz-BTI	train	21.3	20.8192	-0.4808	train	1.1	1.1218	0.0218	train	23.24	23.7344	0.4944
BTORCNA	train	21.1	19.2282	-1.8718	train	1.1	1.1099	0.0099	train	22.84	22.9254	0.0854
MPA-CZ-PTI	train	20.8	20.6149	-0.1851	train	1.07	1.0962	0.0262	train	22.84	22.8684	0.0284
HTM-F	train	20.5	22.7403	2.2403	train	1.09	1.1039	0.0139	train	23.03	23.065	0.035
N01	train	20.4	18.628	-1.772	train	1.08	1.086	0.006	train	23.65	23.4852	-0.1648
BTF6	train	20.3	16.854	-3.446	train	1.13	1.0505	-0.0795	train	22.23	21.1777	-1.0523
TPA-FO	train	20.2	19.5266	-0.6734	train	1.09	1.0407	-0.0493	train	22.76	22.3817	-0.3783
BTORA	test	20.2	18.5789	-1.6211	train	1.09	1.131	0.041	train	22.1	22.5987	0.4987
MCZ-PA-PTI	test	20	20.5523	0.5523	train	1.08	1.1097	0.0297	train	22.66	23.4954	0.8354
HTM-H	train	19	19.492	0.492	train	1.05	1.1133	0.0633	train	22.7	22.3928	-0.3072
N02	train	18.9	17.4714	-1.4286	train	1.03	1.0363	0.0063	train	23.48	23.156	-0.324
BTRA	train	18.4	17.4402	-0.9598	train	1.06	1.074	0.014	test	21.64	21.9771	0.3371
MPA-PA-BTI	train	17.4	19.6867	2.2867	test	0.99	1.0479	0.0579	train	22.15	22.2812	0.1313
TPA-PDO	train	17	19.6477	2.6477	train	1.03	1.0175	-0.0125	train	20.44	22.3833	1.9433
TPADPP-Boc	train	16.3	16.8979	0.5979	train	1.02	1.013	-0.007	train	22.22	22.6217	0.4017
BTF5	train	11.4	17.8568	6.4568	train	0.8	0.9518	0.1518	train	21.31	21.863	0.553

Table (S4): Experimental and predicted PCE, V_{OC}, and J_{SC} values for the test and train sets for dopant free HTMs when used in **PSCs** devices utilizing 1D, and 2D descriptors.

HTM	**PCE**				V_{OC}				J_{SC}			
	Set	Y (Obs)	Y (Pred)	Error	Set	Y (Obs)	Y (Pred)	Error	Set	Y (Obs)	Y(Pred)	Error
TAT-2T-CAN	train	20.1	17.1375	-2.9625	test	1.13	1.0599	-0.0701	train	23.1	22.451	-0.649
C-CPDT	train	19.6	17.6714	-1.9286	train	1.14	1.0609	-0.0791	train	23.27	22.2353	-1.0347
FBA3	train	19.27	17.7561	-1.5139	train	1.09	1.0342	-0.0558	train	22.12	22.4364	0.3164
FBA2	train	18.7	17.7305	-0.9695	train	1.06	1.0334	-0.0266	test	22.32	22.438	0.118
CJ-01	train	18.56	18.0197	-0.5403	train	1.113	1.0604	-0.0526	train	22.32	22.3488	0.0288
TPA-BPFN-TPA	train	18.4	18.1565	-0.2435	train	1.04	1.0461	0.0061	train	22.7	22.3728	-0.3272
ACE-QA-ACE	train	18.2	18.55	0.35	train	1.06	1.065	0.005	train	22.41	22.786	0.376
PCA-1	train	18.17	16.3169	-1.8531	train	1.062	1.0138	-0.0482	test	22.3	22.2235	-0.0765
IDF-SFXPh	train	17.6	17.7639	0.1639	train	1.05	1.0691	0.0191	train	21.5	21.9826	0.4826
BTDTP	train	17.6	17.6993	0.0993	train	0.97	1.0531	0.0831	train	25.73	22.1415	-3.5885
TPA-3T-DCV	train	17.6	16.9618	-0.6382	test	1.08	1.0646	-0.0154	train	23	22.0851	-0.9149
TAT-2T-DCV	test	17.6	16.3725	-1.2276	train	1.08	1.0515	-0.0285	test	23	22.359	-0.641
TPA-ANT-TPA	test	17.5	18.8982	1.3982	train	1.03	1.0744	0.0444	train	21.07	22.2705	1.2005
BTPA-TCNE	train	16.94	17.1599	0.2199	train	1.04	1.0561	0.0161	train	20.84	22.4661	1.6261
BTBDT	train	16.9	17.1932	0.2932	train	0.95	1.0551	0.1051	train	24.68	22.1318	-2.5482

FBA1	test	16.8	17.8444	1.0444	test	1.05	1.0372	-0.0128	train	21.57	22.5089	0.9389
Z1011	train	16.3	16.535	0.235	train	1.096	1.0504	-0.0456	train	20.52	21.8216	1.3016
Z34	test	16.1	18.2365	2.1365	train	1.055	1.0785	0.0235	train	21.245	22.2367	0.9917
CQ2	train	15.2	17.2321	2.0321	test	1.02	1.0286	0.0086	test	20.57	22.4703	1.9003
DTBT	train	11.6	16.9435	5.3435	test	0.93	1.0327	0.1027	test	22.2	22.4774	0.2774
DTBS	test	15	17.5549	2.5549	train	0.96	1.0344	0.0744	train	22.78	22.7024	-0.0776
DOR3T-TBDT	train	14.9	14.5923	-0.3077	test	0.97	1	0.03	train	20.7	21.5859	0.8859
X25	train	14.4	17.6577	3.2577	train	1.01	1.0532	0.0432	train	19.64	22.6608	3.0208
HTM1	train	13.4	17.2828	3.8828	test	0.971	1.0622	0.0912	test	19.3	21.7085	2.4085
DTBF	train	13.3	16.9818	3.6818	train	0.95	1.0286	0.0786	test	22.48	22.4696	-0.0104
T-CPDT	train	11.4	17.597	6.197	train	0.88	1.0671	0.1871	train	21.37	22.1928	0.8228
DFBT-MTP	train	21.2	18.5914	-2.6086	train	1.16	1.0655	-0.0945	train	22.15	22.332	0.182
MPA-BTTI	train	21.17	18.5272	-2.6428	train	1.12	1.0718	-0.0482	train	23.23	22.6115	-0.6185
DBTMT	train	21.1	18.9011	-2.1989	train	1.12	1.0712	-0.0488	test	22.7	22.3642	-0.3358
TPE-S	train	21	18.796	-2.204	test	1.13	1.1018	-0.0282	train	23.3	21.7812	-1.5188
DFH	test	20.6	17.0013	-3.5987	train	1.09	1.0327	-0.0573	train	22.7	22.1126	-0.5874
DBFMT	train	20.5	17.6838	-2.8162	train	1.07	1.0445	-0.0255	train	23.7	22.4097	-1.2903
DPh-DNTT	train	20.1	17.6262	-2.4738	train	1.1	1.0374	-0.0626	train	22.56	22.1334	-0.4266
BT-MTP	test	20.1	18.379	-1.721	train	1.1	1.056	-0.044	train	23.01	22.3071	-0.7029
YJ01	train	19.8	17.7207	-2.0793	train	1.08	1.0338	-0.0462	train	22.53	22.3303	-0.1997
BDT-POZ	train	19.16	19.8416	0.6816	train	1.04	1.0742	0.0342	train	22.56	23.1275	0.5675
FMT	train	19.06	17.3159	-1.7441	train	1.07	1.0423	-0.0277	train	22.52	22.3433	-0.1767
TAPC	train	18.8	17.6908	-1.1092	test	1.04	1.039	-0.001	train	22.32	22.4935	0.1735
XY1	train	18.78	17.8952	-0.8848	train	1.11	1.0745	-0.0355	train	22.21	22.2458	0.0358
VB-MeO-FDPA	train	18.7	17.0991	-1.6009	train	1.15	1.0352	-0.1148	test	20.89	22.0328	1.1428
Trux-OMeTAD	train	18.6	17.8776	-0.7224	train	1.02	1.0925	0.0725	train	23.2	21.9398	-1.2602
H2	test	18.6	18.1436	-0.4564	test	1.06	1.064	0.004	train	22.93	22.2744	-0.6556
D106	test	18.2	18.2567	0.0567	train	1.05	1.0773	0.0273	train	22.32	22.4334	0.1134
m-MTDATA	train	18.12	18.0106	-0.1094	train	1.035	1.0822	0.0472	train	22.5	22.1813	-0.3187
TPAC3M	train	17.54	18.1955	0.6555	train	1	1.0551	0.0551	train	22.79	22.6244	-0.1656
YJ02	train	17.5	17.6868	0.1868	train	1.04	1.0337	-0.0063	train	22.22	22.2685	0.0485
D105	train	17.4	18.9369	1.5369	test	1.04	1.0764	0.0364	train	21.96	22.5842	0.6242
TPA-2,7-FLTPA-TPA	train	17.1	17.4806	0.3806	test	1.052	1.0637	0.0117	train	20.82	21.9077	1.0877
TTA	train	16.7	18.0639	1.3639	train	1.04	1.079	0.039	train	20.4	21.8451	1.4451
TPP-SMeTAD	train	16.6	18.9487	2.3486	train	1.07	1.1002	0.0302	test	20.15	21.8979	1.7479
TPA-TVT-TPA	train	16.32	17.7767	1.4566	test	1.07	1.0334	-0.0366	train	21.49	22.4506	0.9606

D104	train	16.2	19.1411	2.9411	train	1.05	1.0696	0.0196	test	21.22	22.5382	1.3182
CzPAF-TPA	train	15.71	16.5117	0.8017	train	1.05	1.05	0	train	20	21.9266	1.9266
TBDI	train	15.33	17.6513	2.3213	train	1.09	1.0542	-0.0358	train	19.3	22.5194	3.2194
H0	train	13.3	17.3479	4.0479	train	1.02	1.039	0.019	train	22.87	22.195	-0.675
YZ22	train	22.4	18.4496	-3.9504	train	1.1	1.0421	-0.0579	train	25.1	22.4065	-2.6935
SFDT-TMD	train	21.7	17.4526	-4.2474	train	1.13	1.0361	-0.0939	test	24.1	22.2121	-1.8879
MeOTTVT	train	21.3	18.1336	-3.1664	train	1.11	1.0803	-0.0297	train	23.89	22.1945	-1.6955
DTP-C6Th	train	21.04	17.319	-3.721	test	1.15	1.0384	-0.1116	test	22.76	22.425	-0.335
TQ4	test	21	17.6145	-3.3855	train	1.12	1.0401	-0.0799	train	23.71	22.4464	-1.2636
Cz-As	train	20.9	17.8876	-3.0124	train	1.08	1.0612	-0.0188	train	24.4	22.6392	-1.7608
DTPC13-ThTPA	train	20.38	17.0677	-3.3123	train	1.13	1.0341	-0.0959	train	22.82	22.4495	-0.3705
TTE-2	test	20.04	17.9448	-2.0952	train	1.11	1.0847	-0.0253	train	23.26	21.9674	-1.2926
ZT-H2	train	19.6	16.7616	-2.8384	train	1.11	1.0406	-0.0694	train	24.15	22.0717	-2.0783
CuPc	train	19.6	18.1965	-1.4035	train	1.1	1.0646	-0.0354	test	23.96	22.9242	-1.0358
H2Pc	train	19.6	16.9761	-2.6239	test	1.11	1.0313	-0.0787	train	23.85	22.3335	-1.5165
WH-1	test	19.5	17.5169	-1.9831	train	1.08	1.0626	-0.0174	test	23.37	22.3435	-1.0265
YN2	train	19.27	17.8111	-1.4589	train	1.11	1.0532	-0.0568	train	22.87	22.4235	-0.4465
WH-3	test	19.2	18.2081	-0.9919	train	1.07	1.0834	0.0134	train	23.05	22.3787	-0.6713
tpa-t-FBTD	train	18.9	17.7899	-1.1101	test	1.08	1.0411	-0.0389	train	22.4	22.3396	-0.0604
FA-CN	test	18.9	16.4085	-2.4915	train	1.13	1.0755	-0.0545	train	21.71	22.0371	0.3271
Y6-T	train	18.8	16.7177	-2.0823	train	1.1	1.0542	-0.0458	train	22.9	21.9256	-0.9744
Cz-Py	train	18.2	17.4752	-0.7248	train	1.13	1.0489	-0.0811	train	21.9	22.5021	0.6021
YZ18	train	18.1	17.9105	-0.1895	train	1.03	1.0436	0.0136	train	24.1	22.4981	-1.6019
C202	train	17.7	17.5202	-0.1798	train	1.05	1.0397	-0.0103	train	23	22.3992	-0.6008
α,β-COTh-Ph-OMeTAD	train	17.2	15.9327	-1.2673	train	1.05	1.0304	-0.0196	test	21.51	21.2086	-0.3014
C302	train	16.4	16.7184	0.3184	train	1.01	1.0214	0.0114	train	23.3	22.438	-0.862
PhCz-4MeOTPA	train	16	17.4921	1.4921	train	1.08	1.0651	-0.0149	train	21.52	21.897	0.377
X62	train	15.9	18.341	2.441	train	1.01	1.0838	0.0738	train	22.4	21.9618	-0.4382
Spiro-IA	test	15.7	16.8373	1.1373	train	1.04	1.04	0	train	22.14	21.9853	-0.1547
WH-2	train	15.3	17.1257	1.8257	train	1.02	1.0328	0.0128	train	21.95	22.4056	0.4556
2 DBT(QT-TPA)2	test	13.6	15.7395	2.1395	train	1.04	1.0235	-0.0165	train	19.23	21.6352	2.4052
T(EDOT-TPA)2	train	12.3	16.5504	4.2504	train	1.04	1.0389	-0.0011	train	20.25	22.3104	2.0604
TQ3	test	10.8	17.4851	6.6851	train	0.95	1.0375	0.0875	train	20.9	22.3048	1.4048
ZT-H1	train	10	16.9987	6.9987	train	1	1.0477	0.0477	train	21.21	21.9879	0.7779
DT-BT	train	7.3	17.7805	10.4805	train	0.83	1.0405	0.2105	train	16.8	22.2657	5.4657
C301	train	5.8	15.9461	10.1461	train	0.73	0.9941	0.2641	train	19.6	22.3158	2.7158

TPADPP	train	21.6	17.6122	-3.9878	train	1.12	1.0274	-0.0926	train	23.72	22.2176	-1.5024
MCz-cz-BTI	test	21.3	18.364	-2.936	train	1.1	1.0675	-0.0325	test	23.24	21.8874	-1.3526
BTORCNA	test	21.1	17.904	-3.196	test	1.1	1.0498	-0.0502	train	22.84	22.3934	-0.4466
MPA-CZ-PTI	train	20.8	17.8141	-2.9859	train	1.07	1.0688	-0.0012	test	22.84	21.8892	-0.9508
HTM-F	train	20.5	18.4842	-2.0158	test	1.09	1.0789	-0.0111	test	23.03	22.117	-0.913
N01	train	20.4	19.8506	-0.5494	train	1.08	1.08	0	train	23.65	22.968	-0.682
BTF6	train	20.3	17.577	-2.723	train	1.13	1.0237	-0.1063	train	22.23	22.1741	-0.0559
TPA-FO	train	20.2	18.4615	-1.7385	train	1.09	1.0599	-0.0301	train	22.76	22.4086	-0.3514
BTORA	train	20.2	18.1843	-2.0157	test	1.09	1.0561	-0.0339	train	22.1	22.3721	0.2721
MCZ-PA-PTI	train	20	17.0197	-2.9803	train	1.08	1.0481	-0.0319	train	22.66	21.7324	-0.9276
HTM-H	train	19	17.9403	-1.0597	train	1.05	1.0554	0.0054	train	22.7	22.4671	-0.2329
N02	train	18.9	17.2033	-1.6967	train	1.03	1.0429	0.0129	train	23.48	22.5658	-0.9142
BTRA	train	18.4	18.2132	-0.1868	train	1.06	1.0544	-0.0056	test	21.64	22.2491	0.6091
MPA-PA-BTI	test	17.4	17.5194	0.1194	train	0.99	1.0709	0.0809	train	22.15	21.7663	-0.3837
TPA-PDO	train	17	18.1393	1.1393	train	1.03	1.0474	0.0174	train	20.44	22.1957	1.7557
TPADPP-Boc	train	16.3	17.8918	1.5918	test	1.02	1.0586	0.0386	train	22.22	21.9474	-0.2726
BTF5	train	11.4	17.617	6.217	train	0.8	1.0267	0.2267	train	21.31	22.3011	0.9911

Table (S5): Experimental and predicted PCE, V_{OC}, and J_{SC} values for the test and train sets for dopant free HTMs when used in **PSCs** devices utilizing 1D, 2D, and 3D descriptors.

HTM	**PCE**				V_{OC}				J_{SC}			
	Set	Y (Obs)	Y (Pred)	Error	Set	Y (Obs)	Y (Pred)	Error	Set	Y (Obs)	Y(Pred)	Error
TAT-2T-CAN	train	20.1	17.84	-2.26	train	1.13	1.0906	-0.0394	test	23.1	23.0939	-0.0061
C-CPDT	test	19.6	16.8522	-2.7478	train	1.14	1.0257	-0.1143	train	23.27	22.7791	-0.4909
FBA3	train	19.27	16.2876	-2.9824	train	1.09	1.1081	0.0181	train	22.12	21.2395	-0.8805
FBA2	test	18.7	17.0017	-1.6983	train	1.06	1.0267	-0.0333	train	22.32	21.9678	-0.3522
CJ-01	train	18.56	18.2303	-0.3297	train	1.113	1.0398	-0.0732	train	22.32	22.3567	0.0367
TPA-BPFN-TPA	train	18.4	19.6392	1.2392	train	1.04	1.0362	-0.0038	train	22.7	22.5361	-0.1639
ACE-QA-ACE	train	18.2	19.6709	1.4709	train	1.06	1.0511	-0.0089	train	22.41	22.6626	0.2526
PCA-1	train	18.17	17.5958	-0.5742	test	1.062	1.0604	-0.0016	test	22.3	22.5506	0.2506
IDF-SFXPh	test	17.6	19.1629	1.5629	test	1.05	1.0661	0.0161	test	21.5	21.9021	0.4021
BTDTP	train	17.6	17.7441	0.1441	train	0.97	0.9962	0.0262	train	25.73	24.6318	-1.0982
TPA-3T-DCV	train	17.6	17.7851	0.1851	test	1.08	1.1032	0.0232	test	23	21.5881	-1.4119
TAT-2T-DCV	train	17.6	18.0968	0.4968	train	1.08	1.1306	0.0506	train	23	22.7651	-0.2349
TPA-ANT-TPA	train	17.5	18.1405	0.6405	test	1.03	1.0329	0.0029	train	21.07	21.7607	0.6907
BTPA-TCNE	train	16.94	18.7225	1.7825	test	1.04	1.0577	0.0177	train	20.84	20.9597	0.1197
BTBDT	train	16.9	17.0065	0.1065	train	0.95	0.9754	0.0254	test	24.68	24.2187	-0.4613

FBA1	test	16.8	16.9029	0.1029	train	1.05	0.9917	-0.0583	train	21.57	22.1483	0.5783
Z1011	train	16.3	16.9973	0.6973	train	1.096	1.0982	0.0022	test	20.52	21.3442	0.8242
Z34	train	16.1	18.5076	2.4076	train	1.055	1.0788	0.0238	train	21.245	21.8593	0.6143
CQ2	train	15.2	16.9299	1.7299	train	1.02	1.0118	-0.0082	train	20.57	22.3333	1.7633
DTBT	train	11.6	16.1575	4.5575	train	0.93	1.0035	0.0735	test	22.2	22.7782	0.5782
DTBS	train	15	14.6568	-0.3432	train	0.96	0.9236	-0.0364	train	22.78	22.5593	-0.2207
DOR3T-TBDT	train	14.9	13.8247	-1.0753	train	0.97	0.981	0.011	train	20.7	21.1269	0.4269
X25	train	14.4	18.317	3.917	train	1.01	1.0401	0.0301	train	19.64	22.4282	2.7882
HTM1	train	13.4	17.0789	3.6789	train	0.971	1.027	0.056	train	19.3	21.1826	1.8826
DTBF	test	13.3	15.8082	2.5082	test	0.95	0.9987	0.0487	train	22.48	22.7469	0.2669
T-CPDT	train	11.4	16.3525	4.9525	train	0.88	0.9781	0.0981	train	21.37	22.1823	0.8123
DFBT-MTP	test	21.2	20.8781	-0.3219	test	1.16	1.1371	-0.0229	train	22.15	22.461	0.311
MPA-BTTI	train	21.17	20.153	-1.017	train	1.12	1.088	-0.032	train	23.23	23.4341	0.2041
DBTMT	test	21.1	20.7475	-0.3525	train	1.12	1.1335	0.0135	train	22.7	22.8052	0.1052
TPE-S	train	21	20.0411	-0.9589	train	1.13	1.1082	-0.0218	train	23.3	22.102	-1.198
DFH	train	20.6	19.9806	-0.6194	train	1.09	1.062	-0.028	test	22.7	22.6565	-0.0435
DBFMT	test	20.5	20.6025	0.1025	train	1.07	1.1063	0.0363	test	23.7	22.9859	-0.7141
DPh-DNTT	train	20.1	16.8759	-3.2241	train	1.1	1.0992	-0.0008	train	22.56	21.4517	-1.1083
BT-MTP	train	20.1	21.1408	1.0408	train	1.1	1.1487	0.0487	train	23.01	23.0245	0.0145
YJ01	train	19.8	19.2941	-0.5059	train	1.08	1.0527	-0.0273	train	22.53	22.7807	0.2507
BDT-POZ	test	19.16	18.3455	-0.8145	train	1.04	1.0873	0.0473	train	22.56	23.0142	0.4542
FMT	train	19.06	19.2852	0.2252	test	1.07	1.0784	0.0084	train	22.52	22.2822	-0.2378
TAPC	train	18.8	17.7656	-1.0344	train	1.04	0.9903	-0.0497	test	22.32	21.6567	-0.6633
XY1	train	18.78	17.1123	-1.6677	train	1.11	1.0527	-0.0573	train	22.21	22.0633	-0.1467
VB-MeO-FDPA	train	18.7	18.6936	-0.0064	train	1.15	1.0998	-0.0502	train	20.89	21.3757	0.4856
Trux-OMeTAD	train	18.6	17.7108	-0.8892	train	1.02	0.9976	-0.0224	train	23.2	21.1991	-2.0009
H2	train	18.6	18.8642	0.2642	train	1.06	1.0724	0.0124	train	22.93	23.8454	0.9154
D106	train	18.2	18.8329	0.6329	train	1.05	1.0653	0.0153	train	22.32	22.5453	0.2253
m-MTDATA	train	18.12	17.7107	-0.4093	train	1.035	1.0103	-0.0247	test	22.5	21.273	-1.227
TPAC3M	train	17.54	17.5643	0.0243	train	1	1.0002	0.0002	train	22.79	22.0835	-0.7065
YJ02	train	17.5	18.8842	1.3842	train	1.04	1.041	0.001	train	22.22	22.5006	0.2806
D105	train	17.4	17.5097	0.1097	train	1.04	1.0268	-0.0132	test	21.96	22.2199	0.2599
TPA-2,7-FLTPA-TPA	train	17.1	16.8735	-0.2265	test	1.052	1.0036	-0.0484	train	20.82	20.818	-0.002
TTA	test	16.7	17.5398	0.8398	test	1.04	1.0123	-0.0277	train	20.4	19.2233	-1.1767
TPP-SMeTAD	train	16.6	19.7407	3.1407	train	1.07	1.0987	0.0287	train	20.15	21.9147	1.7647
TPA-TVT-TPA	train	16.32	17.3811	1.0611	train	1.07	1.0598	-0.0102	train	21.49	22.6621	1.1721
D104	train	16.2	17.0321	0.8321	train	1.05	1.0483	-0.0017	train	21.22	21.6989	0.4789

CzPAF-TPA	train	15.71	16.8641	1.1541	train	1.05	1.0021	-0.0479	train	20	21.2896	1.2896
TBDI	test	15.33	14.4938	-0.8362	test	1.09	1.0224	-0.0676	train	19.3	19.9342	0.6342
H0	train	13.3	15.8171	2.5171	train	1.02	1.0311	0.0111	test	22.87	22.3919	-0.4781
YZ22	train	22.4	18.7046	-3.6954	train	1.1	1.0217	-0.0783	train	25.1	22.9565	-2.1436
SFDT-TMD	train	21.7	19.7081	-1.9919	test	1.13	1.067	-0.063	train	24.1	22.6648	-1.4352
MeOTTVT	train	21.3	18.6244	-2.6756	test	1.11	1.0751	-0.0349	train	23.89	22.0576	-1.8324
DTP-C6Th	train	21.04	18.5835	-2.4565	train	1.15	1.1334	-0.0166	train	22.76	22.7184	-0.0416
TQ4	train	21	17.2372	-3.7628	test	1.12	1.0414	-0.0786	train	23.71	23.246	-0.464
Cz-As	train	20.9	20.439	-0.461	train	1.08	1.1015	0.0215	train	24.4	23.4136	-0.9864
DTPC13-ThTPA	train	20.38	16.453	-3.927	train	1.13	1.0815	-0.0485	test	22.82	22.6403	-0.1797
TTE-2	train	20.04	18.0391	-2.0009	train	1.11	1.086	-0.024	train	23.26	21.8396	-1.4204
ZT-H2	train	19.6	15.7737	-3.8263	train	1.11	1.064	-0.046	train	24.15	22.0849	-2.0651
CuPc	train	19.6	18.8531	-0.7469	test	1.1	1.0534	-0.0466	test	23.96	21.9531	-2.0069
H2Pc	train	19.6	17.3315	-2.2685	train	1.11	1.121	0.011	train	23.85	22.8528	-0.9972
WH-1	train	19.5	19.5309	0.0309	train	1.08	1.0645	-0.0155	train	23.37	22.6754	-0.6946
YN2	train	19.27	17.4021	-1.8679	test	1.11	1.0732	-0.0368	train	22.87	22.6806	-0.1894
WH-3	train	19.2	16.6713	-2.5287	train	1.07	1.0864	0.0164	train	23.05	21.8803	-1.1697
tpa-t-FBTD	train	18.9	16.9567	-1.9433	train	1.08	1.0266	-0.0534	train	22.4	23.1308	0.7308
FA-CN	test	18.9	19.5876	0.6876	train	1.13	1.1532	0.0232	train	21.71	21.53	-0.18
Y6-T	train	18.8	15.5075	-3.2925	train	1.1	1.0928	-0.0072	train	22.9	22.5403	-0.3597
Cz-Py	test	18.2	20.0116	1.8116	train	1.13	1.1057	-0.0243	train	21.9	23.2543	1.3543
YZ18	test	18.1	18.5403	0.4403	train	1.03	1.0352	0.0052	train	24.1	22.4507	-1.6493
C202	train	17.7	17.6356	-0.0644	train	1.05	1.0291	-0.0209	train	23	22.9556	-0.0444
α,β-COTh-Ph-OMeTAD	test	17.2	16.8012	-0.3988	train	1.05	1.0188	-0.0312	train	21.51	20.8186	-0.6914
C302	train	16.4	12.2762	-4.1238	train	1.01	0.9072	-0.1028	test	23.3	21.9854	-1.3146
PhCz-4MeOTPA	train	16	15.4824	-0.5176	test	1.08	1.0029	-0.0771	train	21.52	20.7869	-0.7331
X62	test	15.9	18.6638	2.7638	test	1.01	1.0405	0.0305	train	22.4	21.5913	-0.8087
Spiro-IA	train	15.7	14.3834	-1.3166	train	1.04	1.0452	0.0052	train	22.14	21.5059	-0.6341
WH-2	train	15.3	14.9147	-0.3853	train	1.02	1.0417	0.0217	train	21.95	21.411	-0.539
2 DBT(QT-TPA)2	test	13.6	14.2028	0.6028	train	1.04	1.0427	0.0027	train	19.23	20.3705	1.1405
T(EDOT-TPA)2	train	12.3	12.3241	0.0241	train	1.04	1.0745	0.0345	test	20.25	22.0697	1.8197
TQ3	train	10.8	16.2291	5.4291	test	0.95	1.0282	0.0782	test	20.9	22.6321	1.7321
ZT-H1	test	10	15.1285	5.1285	train	1	1.041	0.041	train	21.21	21.3622	0.1522
DT-BT	train	7.3	15.6395	8.3395	train	0.83	0.9495	0.1195	train	16.8	21.7515	4.9515
C301	train	5.8	11.3253	5.5253	train	0.73	0.8739	0.1439	test	19.6	21.6795	2.0795

TPADPP	train	21.6	19.2428	-2.3572	train	1.12	1.0805	-0.0395	train	23.72	23.3672	-0.3528
MCz-cz-BTI	train	21.3	20.9113	-0.3887	train	1.1	1.1098	0.0098	train	23.24	23.5737	0.3337
BTORCNA	train	21.1	19.3324	-1.7676	train	1.1	1.1142	0.0142	train	22.84	23.0195	0.1795
MPA-CZ-PTI	train	20.8	20.5569	-0.2431	train	1.07	1.0919	0.0219	train	22.84	22.8074	-0.0326
HTM-F	train	20.5	22.9984	2.4984	train	1.09	1.1257	0.0357	train	23.03	22.9764	-0.0536
N01	train	20.4	18.9502	-1.4498	train	1.08	1.0951	0.0151	train	23.65	23.4081	-0.2419
BTF6	train	20.3	16.8816	-3.4184	train	1.13	1.0508	-0.0792	train	22.23	21.2343	-0.9957
TPA-FO	train	20.2	19.6323	-0.5677	train	1.09	1.0249	-0.0651	train	22.76	22.2937	-0.4663
BTORA	test	20.2	18.7721	-1.4279	train	1.09	1.1238	0.0338	train	22.1	22.6237	0.5237
MCZ-PA-PTI	test	20	20.306	0.306	train	1.08	1.0973	0.0173	train	22.66	23.2832	0.6232
HTM-H	train	19	19.4982	0.4982	train	1.05	1.1178	0.0678	train	22.7	22.5816	-0.1184
N02	train	18.9	17.6962	-1.2037	train	1.03	1.0497	0.0197	train	23.48	23.2862	-0.1938
BTRA	train	18.4	17.7665	-0.6335	train	1.06	1.0704	0.0104	test	21.64	21.8248	0.1848
MPA-PA-BTI	train	17.4	19.4976	2.0976	test	0.99	1.0434	0.0534	train	22.15	22.1412	-0.0088
TPA-PDO	train	17	19.4742	2.4742	train	1.03	1.003	-0.027	train	20.44	22.2352	1.7952
TPADPP-Boc	train	16.3	16.6315	0.3315	train	1.02	0.9765	-0.0435	train	22.22	22.5766	0.3566
BTF5	train	11.4	17.7647	6.3647	train	0.8	0.9651	0.1651	train	21.31	21.9117	0.6017

Table (S6): Experimental and predicted PCE, V_{OC}, and J_{SC} values for the test and train sets for dopant free HTMs when used in **PSCs** devices utilizing 2D binary fingerprints descriptors.

HTM	**PCE**				V_{OC}				J_{SC}			
	Set	Y (Obs)	Y (Pred)	Error	Set	Y (Obs)	Y (Pred)	Error	Set	Y (Obs)	Y (Pred)	Error
TAT-2T-CAN	train	20.1	17.7501	-2.3499	train	1.13	1.1525	0.0225	test	23.1	22.1477	-0.9523
C-CPDT	train	19.6	16.7381	-2.8619	train	1.14	1.0685	-0.0715	train	23.27	22.5107	-0.7593
FBA3	train	19.27	18.1646	-1.1054	train	1.09	1.1613	0.0713	train	22.12	21.7637	-0.3563
FBA2	test	18.7	17.9406	-0.7594	test	1.06	1.087	0.027	train	22.32	21.8508	-0.4692
CJ-01	train	18.56	18.9603	0.4003	train	1.113	1.0634	-0.0496	train	22.32	22.1532	-0.1668
TPA-BPFN-TPA	train	18.4	19.3235	0.9235	train	1.04	1.0254	-0.0146	train	22.7	22.1005	-0.5995
ACE-QA-ACE	test	18.2	17.2422	-0.9578	train	1.06	1.0728	0.0128	train	22.41	22.1937	-0.2163
PCA-1	train	18.17	17.7415	-0.4285	test	1.062	1.0441	-0.0179	test	22.3	22.8069	0.5069
IDF-SFXPh	train	17.6	16.729	-0.871	test	1.05	1.0151	-0.0349	test	21.5	22.2906	0.7906
BTDTP	train	17.6	16.001	-1.598	train	0.97	0.954	-0.0151	train	25.73	25.1494	-0.5806
TPA-3T-DCV	train	17.6	17.553	-0.046	train	1.08	1.058	-0.021	test	23	22.4031	-0.5969
TAT-2T-DCV	train	17.6	16.783	-0.817	train	1.08	1.096	0.0164	train	23	22.2397	-0.7603
TPA-ANT-TPA	train	17.5	16.139	-1.36	train	1.03	1.011	-0.0181	train	21.07	21.9372	0.8672
BTPA-TCNE	train	16.94	19.043	2.1034	train	1.04	1.021	-0.0184	train	20.84	21.5164	0.6764
BTBDT	test	16.9	15.9625	-0.9375	train	0.95	0.952	0.0026	test	24.68	24.2794	-0.4006

FBA1	train	16.8	15.526	-1.273	train	1.05	1.019	-0.031	train	21.57	21.3169	-0.2531
Z1011	train	16.3	18.066	1.7668	train	1.096	1.08	-0.0155	test	20.52	21.9734	1.4534
Z34	train	16.1	19.191	3.0912	train	1.055	1.079	0.0241	train	21.245	22.305	1.06
CQ2	train	15.2	15.887	0.6877	test	1.02	1.034	0.014	train	20.57	20.6785	0.1085
DTBT	train	11.6	13.395	1.795	test	0.93	0.9741	0.0441	test	22.2	23.1951	0.9951
DTBS	test	15	13.6621	-1.3379	train	0.96	0.974	0.0141	train	22.78	23.1951	0.4151
DOR3T-TBDT	train	14.9	14.009	-0.89	train	0.97	0.972	0.0024	train	20.7	21.0294	0.3294
X25	train	14.4	16.24	1.8409	train	1.01	1.022	0.0127	train	19.64	21.1655	1.5255
HTM1	train	13.4	15.483	2.0836	train	0.971	0.959	-0.0112	train	19.3	21.4956	2.1956
DTBF	test	13.3	13.7587	0.4587	test	0.95	0.9741	0.0241	train	22.48	22.9777	0.4977
T-CPDT	train	11.4	13.941	2.5415	train	0.88	0.972	0.0929	train	21.37	21.8431	0.4731
DFBT-MTP	train	21.2	21.054	-0.146	test	1.16	1.1541	-0.0059	train	22.15	22.4525	0.3025
MPA-BTTI	train	21.17	19.128	-2.041	train	1.12	1.129	0.009	train	23.23	23.3764	0.1464
DBTMT	train	21.1	21.259	0.1596	test	1.12	1.067	-0.053	train	22.7	22.2614	-0.4386
TPE-S	train	21	20.565	-0.434	test	1.13	1.0712	-0.0588	train	23.3	22.1563	-1.1437
DFH	test	20.6	20.8659	0.2659	train	1.09	1.091	0.001	test	22.7	22.3998	-0.3002
DBFMT	train	20.5	21.916	1.416	train	1.07	1.067	-0.003	test	23.7	22.6189	-1.0811
DPh-DNTT	test	20.1	17.3029	-2.7971	train	1.1	1.089	-0.0103	train	22.56	22.6285	0.0685
BT-MTP	train	20.1	20.832	0.7327	train	1.1	1.104	0.0046	train	23.01	22.4773	-0.5327
YJ01	train	19.8	19.323	-0.477	train	1.08	1.066	-0.0134	train	22.53	22.0949	-0.4352
BDT-POZ	train	19.16	18.364	-0.795	train	1.04	1.084	0.0442	train	22.56	23.8507	1.2907
FMT	train	19.06	21.156	2.0967	train	1.07	1.074	0.0047	train	22.52	22.493	-0.027
TAPC	test	18.8	20.4525	1.6525	train	1.04	1.007	-0.0329	test	22.32	22.2717	-0.0483
XY1	train	18.78	17.528	-1.251	train	1.11	1.125	0.0153	train	22.21	22.1543	-0.0557
VB-MeO-FDPA	train	18.7	20.223	1.5237	train	1.15	1.151	0.0012	train	20.89	22.1268	1.2368
Trux-OMeTAD	train	18.6	18.408	-0.191	train	1.02	1.018	-0.002	train	23.2	22.801	-0.399
H2	train	18.6	16.892	-1.707	train	1.06	1.0858	0.0258	train	22.93	23.3784	0.4484
D106	train	18.2	18.906	0.7068	train	1.05	1.054	0.004	train	22.32	21.7879	-0.5321
m-MTDATA	train	18.12	19.653	1.5336	test	1.035	1.0446	0.0096	test	22.5	21.3248	-1.1752
TPAC3M	train	17.54	18.684	1.1443	train	1	1.029	0.0297	train	22.79	22.2647	-0.5253
YJ02	test	17.5	19.3916	1.8916	train	1.04	1.066	0.0266	train	22.22	21.949	-0.2709
D105	train	17.4	18.609	1.2091	test	1.04	1.054	0.014	test	21.96	21.7828	-0.1772
TPA-2,7-FLTPA-TPA	train	17.1	16.2	-0.899	train	1.052	1.088	0.036	train	20.82	20.7623	-0.0577
TTA	train	16.7	18.015	1.3152	train	1.04	1.056	0.0165	train	20.4	21.6541	1.2541
TPP-SMeTAD	test	16.6	18.3141	1.7141	train	1.07	1.059	-0.0102	train	20.15	21.4308	1.2808
TPA-TVT-TPA	train	16.32	19.132	2.8128	train	1.07	1.076	0.0066	train	21.49	22.0131	0.5231
D104	test	16.2	18.6091	2.4091	train	1.05	1.054	0.004	train	21.22	21.7334	0.5134
CzPAF-TPA	train	15.71	15.54	-0.169	train	1.05	1.034	-0.0157	train	20	20.3492	0.3492
TBDI	train	15.33	17.296	1.9664	train	1.09	1.089	-0.001	train	19.3	20.7175	1.4175

H0	train	13.3	14.243	0.9433	train	1.02	1.005	-0.0144	test	22.87	23.136	0.266
YZ22	train	22.4	19.795	-2.604	test	1.1	1.0671	-0.0329	train	25.1	23.0158	-2.0842
SFDT-TMD	test	21.7	21.1832	-0.5168	train	1.13	1.082	-0.0478	train	24.1	22.9113	-1.1887
MeOTTVT	test	21.3	19.1912	-2.1088	train	1.11	1.079	-0.0309	train	23.89	22.305	-1.585
DTP-C6Th	test	21.04	17.8112	-3.2288	train	1.15	1.162	0.0124	train	22.76	22.7777	0.0177
TQ4	train	21	15.941	-5.058	train	1.12	1.089	-0.0309	train	23.71	21.5126	-2.1974
Cz-As	train	20.9	20.141	-0.758	train	1.08	1.1249	0.0449	train	24.4	23.1566	-1.2433
DTPC13-ThTPA	train	20.38	18.362	-2.017	train	1.13	1.136	0.006	test	22.82	23.2192	0.3992
TTE-2	train	20.04	17.278	-2.761	test	1.11	1.0945	-0.0155	train	23.26	22.887	-0.373
ZT-H2	train	19.6	17.329	-2.27	train	1.11	1.063	-0.0467	train	24.15	23.7128	-0.4372
CuPc	train	19.6	19.737	0.1374	train	1.1	1.089	-0.0106	test	23.96	22.9399	-1.0201
H2Pc	test	19.6	19.9393	0.3392	train	1.11	1.089	-0.0206	train	23.85	22.9106	-0.9394
WH-1	train	19.5	21.06	1.5602	train	1.08	1.054	-0.0257	train	23.37	22.6234	-0.7466
YN2	train	19.27	17.392	-1.877	train	1.11	1.177	0.0671	train	22.87	21.9082	-0.9618
WH-3	test	19.2	18.8878	-0.3122	test	1.07	1.0622	-0.0078	train	23.05	22.1364	-0.9136
tpa-t-FBTD	train	18.9	16.662	-2.237	train	1.08	1.061	-0.0187	train	22.4	21.597	-0.803
FA-CN	train	18.9	16.792	-2.107	train	1.13	1.141	0.0113	train	21.71	20.9562	-0.7538
Y6-T	train	18.8	16.893	-1.906	train	1.1	1.089	-0.0108	train	22.9	23.0279	0.1279
Cz-Py	train	18.2	20.018	1.8184	train	1.13	1.1249	-0.0051	train	21.9	23.1122	1.2122
YZ18	train	18.1	19.823	1.7233	train	1.03	0.9845	-0.0455	train	24.1	21.9921	-2.1079
C202	train	17.7	17.045	-0.654	train	1.05	1.061	0.011	train	23	22.4395	-0.5605
?, ?-COTh-Ph-OMeTAD	train	17.2	15.999	-1.2	test	1.05	1.0613	0.0113	train	21.51	22.979	1.469
C302	train	16.4	15.134	-1.265	train	1.01	0.9268	-0.0832	test	23.3	22.6587	-0.6413
PhCz-4MeOTPA	train	16	19.621	3.6212	train	1.08	1.0614	-0.0186	train	21.52	22.3546	0.8346
X62	train	15.9	15.752	-0.147	train	1.01	1.0019	-0.0081	train	22.4	22.3488	-0.0512
Spiro-IA	train	15.7	14.665	-1.034	train	1.04	1.001	-0.039	train	22.14	21.5486	-0.5914
WH-2	train	15.3	17.738	2.4388	train	1.02	1.071	0.0513	train	21.95	21.7985	-0.1515
2 DBT(QT-TPA)2	train	13.6	13.263	-0.336	train	1.04	1.0526	0.0126	train	19.23	18.9518	-0.2782
T(EDOT-TPA)2	test	12.3	16.682	4.382	train	1.04	1.037	-0.003	test	20.25	21.7804	1.5304
TQ3	train	10.8	11.792	0.9928	train	0.95	0.9738	0.0238	test	20.9	20.8787	-0.0213
ZT-H1	train	10	11.065	1.0655	train	1	1.016	0.0165	train	21.21	21.9698	0.7598
DT-BT	train	7.3	12.6945	5.3945	train	0.83	0.849	0.0195	train	16.8	19.9859	3.1859
C301	train	5.8	8.096	2.296	train	0.73	0.815	0.085	test	19.6	21.58	1.98
TPADPP	train	21.6	19.858	-1.741	train	1.12	1.083	-0.0369	train	23.72	22.6018	-1.1182
MCz-cz-BTI	train	21.3	21.039	-0.26	test	1.1	1.0943	-0.0057	train	23.24	23.9642	0.7242
BTORCNA	train	21.1	18.931	-2.168	train	1.1	1.0798	-0.0202	train	22.84	22.6764	-0.1636

MPA-CZ-PTI	train	20.8	20.763	-0.036	train	1.07	1.045	-0.0247	train	22.84	23.791	0.951
HTM-F	train	20.5	19.037	-1.463	test	1.09	1.1279	0.0379	train	23.03	22.3142	-0.7158
N01	train	20.4	18.883	-1.516	test	1.08	1.0812	0.0012	train	23.65	24.5296	0.8796
BTF6	train	20.3	15.382	-4.917	train	1.13	1.038	-0.092	train	22.23	20.6778	-1.5522
TPA-FO	train	20.2	19.969	-0.23	train	1.09	1.0515	-0.0385	train	22.76	22.1822	-0.5779
BTORA	test	20.2	18.3659	-1.8341	train	1.09	1.1019	0.0119	train	22.1	21.98	-0.12
MCZ-PA-PTI	train	20	20.133	0.1335	train	1.08	1.12	0.022	train	22.66	23.6247	0.9647
HTM-H	train	19	18.503	-0.496	train	1.05	1.0613	0.0113	train	22.7	22.0682	-0.6318
N02	train	18.9	18.772	-0.127	test	1.03	1.0812	0.0512	train	23.48	24.3814	0.9014
BTRA	test	18.4	17.831	-0.568	train	1.06	1.016	0.044	test	21.64	21.1126	-0.5274
MPA-PA-BTI	test	17.4	18.328	0.9283	test	0.99	1.0638	0.0738	train	22.15	23.3278	1.1778
TPA-PDO	train	17	19.82	2.819	train	1.03	1.0551	0.0215	train	20.44	22.1822	1.7421
TPADPP-Boc	train	16.3	18.67	30 2.373	train	1.02	1.0831	0.0631	train	22.22	22.4177	0.1977 TPADPP-Boc
BTF5	train	11.4	13.14	1.744	train	0.8	0.918	0.118	train	21.31	20.6108	-0.6992 BTF5

Table (S7): Experimental and predicted PCE, V_{OC}, and J_{SC} values for the test and train sets for dopant free HTMs when used in conventional n-i-p PSCs based on MALHs utilizing BF descriptors.

HTM	**PCE**				V_{OC}				J_{SC}			
	Set	**Y(Exp)**	**Y(Pred)**	**Error**	**Set**	**Y(Exp)**	**Y(Pred)**	**Error**	**Set**	**Y(Exp)**	**Y(Pred)**	**Error**
TAT–2T–CAN [1]	train	20.1	20.4834	0.3834	train	1.13	1.1479	0.018	test	23.1	22.908	-0.192
C-CPDT [2]	train	19.6	19.2695	-0.3305	train	1.14	1.1052	-0.035	train	23.27	22.8846	-0.385
FBA3 [3]	train	19.27	19.4947	0.2247	train	1.09	1.0674	-0.023	train	22.12	22.5936	0.473
FBA2 [3]	test	18.7	19.0024	0.3024	train	1.06	1.0466	-0.013	train	22.32	22.6893	0.369
CJ-01 [4]	train	18.56	18.0767	-0.4833	train	1.113	1.1138	0.001	train	22.32	21.7373	-0.582
TPA–BPFN–TPA [5]	train	18.4	17.9022	-0.4978	train	1.04	1.0413	0.001	train	22.7	21.8408	-0.859
ACE-QA-ACE [6]	test	18.2	17.3032	-0.8968	train	1.06	1.0559	-0.004	train	22.41	22.3798	-0.030
PCA-1 [7]	train	18.17	18.245	0.075	train	1.062	1.0576	-0.004	train	22.3	21.8148	-0.4852
IDF-SFXPh [8]	train	17.6	17.3834	-0.2166	test	1.05	1.0409	-0.009	train	21.5	21.1616	-0.338
BTDTP [9]	train	17.6	17.1118	-0.4882	train	0.97	0.9622	-0.008	train	25.73	25.8409	0.110
TPA–3T–DCV [1]	test	17.6	16.4801	-1.1199	train	1.08	1.0762	-0.004	train	23	22.642	-0.358
TAT–2T–DCV [1]	train	17.6	17.96	0.36	train	1.08	1.1036	0.024	train	23	23.1368	0.1368
TPA-ANT-TPA [10]	train	17.5	17.548	0.048	train	1.03	1.0284	-0.002	train	21.07	21.1402	0.070
BTPA-TCNE [11]	train	16.94	17.3003	0.3603	train	1.04	1.0699	0.029	train	20.84	21.0275	0.187
BTBDT [12]	train	16.9	16.7598	-0.1402	train	0.95	0.9446	-0.005	test	24.68	24.0683	-0.611
FBA1 [13]	train	16.8	16.5164	-0.2836	train	1.05	1.0328	-0.017	test	21.57	21.7864	0.216

Z1011 [13]	train	16.3	16.0897	-0.2103	test	1.096	1.0554	-0.041	train	20.52	20.9872	0.467
Z34 [14]	test	16.1	16.3975	0.2975	train	1.055	1.0516	-0.003	test	21.245	21.1242	-0.121
CQ2 [15]	train	15.2	14.7716	-0.4284	test	1.02	1.0052	-0.015	train	20.57	20.5786	0.008
DTBT [16]	train	11.6	12.1195	0.5195	test	0.93	0.9391	0.009	train	22.2	22.2487	0.048
DTBS [17]	train	15	13.0839	-1.9161	train	0.96	0.936	-0.024	train	22.78	22.2487	-0.531
DOR3T-TBDT [18]	train	14.9	14.5732	-0.3268	train	0.97	0.9774	0.007	train	20.7	20.6102	-0.089
X25 [15]	train	14.4	15.3435	0.9435	train	1.01	1.0295	0.019	train	19.64	20.305	0.665
HTM1 [19]	train	13.4	12.9748	-0.4252	train	0.971	0.9494	-0.022	train	19.3	19.2772	-0.0228
DTBF [20]	test	13.3	12.6325	-0.6675	test	0.95	0.9391	-0.011	test	22.48	22.2487	-0.2313
T-CPDT [2]	train	11.4	14.2325	2.8325	train	0.88	0.9436	0.064	train	21.37	22.5152	1.145

Table (S8): Experimental and predicted PCE, V_{OC}, and J_{SC} values for the test and train sets for dopant free HTMs when used in inverted p-i-n PSCs based on MALHs utilizing binary fingerprints descriptors.

HTM	**PCE**				**V_{OC}**				**J_{SC}**			
	Set	**Y(Exp)**	**Y(Pred)**	**Error**	**Set**	**Y(Exp)**	**Y(Pred)**	**Error**	**Set**	**Y(Exp)**	**Y(Pred)**	**Error**
DFBT-MTP [21]	train	21.2	21.5444	0.3444	train	1.16	1.1635	0.0035	train	22.15	22.4381	0.288
MPA-BTTI [22]	train	21.17	21.0147	-0.1553	train	1.12	1.1172	-0.003	train	23.23	22.9845	-0.245
DBTMT [23]	train	21.1	22.4515	1.3515	train	1.12	1.1209	0.001	train	22.7	23.3823	0.682
TPE-S [24]	train	21	19.443	-1.557	train	1.13	1.1072	-0.0228	train	23.3	22.5305	-0.769
DFH [25]	train	20.6	20.0505	-0.5495	train	1.09	1.0798	-0.010	train	22.7	22.7236	0.024
DBFMT [26]	train	20.5	20.7531	0.2531	train	1.07	1.068	-0.002	test	23.7	22.8781	-0.822
DPh-DNTT [27]	test	20.1	19.2165	-0.8835	train	1.1	1.1021	0.002	train	22.56	22.2283	-0.332
BT-MTP [28]	train	20.1	19.8603	-0.2397	test	1.1	1.1025	0.002	train	23.01	22.8578	-0.152
YJ01 [29]	train	19.8	18.1978	-1.6022	test	1.08	1.0608	-0.019	train	22.53	22.3546	-0.175
BDT-POZ [30]	train	19.16	19.1307	-0.0293	test	1.04	1.0426	0.003	train	22.56	22.1669	-0.393
FMT [31]	test	19.06	19.5818	0.5218	train	1.07	1.0837	0.014	test	22.52	22.0388	-0.481
TAPC [32]	train	18.8	18.5655	-0.2345	test	1.04	1.0694	0.029	train	22.32	22.521	0.201
XY1 [33]	train	18.78	18.7282	-0.0518	train	1.11	1.1255	0.015	test	22.21	22.0456	-0.164
VB-MeO-FDPA [34]	train	18.7	18.744	0.044	train	1.15	1.1242	-0.026	train	20.89	21.3428	0.453
Trux-OMeTAD [35]	train	18.6	18.4662	-0.1338	train	1.02	1.0094	-0.010	train	23.2	22.9888	-0.211
H2 [36]	train	18.6	18.896	0.296	train	1.06	1.0545	-0.0055	test	22.93	22.9643	0.034
D106 [37]	test	18.2	17.0692	-1.1308	train	1.05	1.0415	-0.008	train	22.32	21.7771	-0.543
m-MTDATA [38]	train	18.12	18.0468	-0.0732	train	1.035	1.0511	0.016	train	22.5	22.5308	0.031
TPAC3M [39]	train	17.54	17.6362	0.0962	train	1	1.0092	0.009	train	22.79	22.5598	-0.230
YJ02 [40]	train	17.5	17.3719	-0.1281	train	1.04	1.0576	0.017	train	22.22	22.1691	-0.051
D105 [37]	train	17.4	17.0692	-0.3308	train	1.04	1.0376	-0.002	train	21.96	21.6733	-0.287
TPA-2,7-FLTPA-TPA [41]	test	17.1	17.1138	0.0138	train	1.052	1.0325	-0.019	test	20.82	21.1628	0.343
TTA [42]	train	16.7	17.2157	0.5157	train	1.04	1.0605	0.020	train	20.4	20.254	-0.146

TPP-SMeTAD [43]	train	16.6	17.5165	0.9165	train	1.07	1.09	0.020	train	20.15	21.0848	0.935
TPA-TVT-TPA [44]	train	16.32	17.0022	0.6822	train	1.07	1.081	0.01	train	21.49	21.9853	0.495
D104 [37]	test	16.2	17.0692	0.8692	train	1.05	1.0412	-0.009	train	21.22	21.6733	0.453
CzPAF-TPA [45]	train	15.71	15.3391	-0.3709	test	1.05	1.0347	-0.015	train	20	19.9852	-0.015
TBDI [46]	train	15.33	14.8467	-0.4833	train	1.09	1.0735	-0.0165	train	19.3	19.0653	-0.2347
H0 [36]	train	13.3	14.7398	1.4398	train	1.02	1.0253	0.0053	train	22.87	23.0925	0.2225

Table (S9): Experimental and predicted PCE, V_{OC}, and J_{SC} values for the test and train sets for dopant free HTMs when used in conventional (n-i-p) PSCs based on mixed CLHs.

HTM	PCE				V_{OC}				J_{SC}			
	Set	Y(Exp)	Y(Pred)	Error	Set	Y(Exp)	Y(Pred)	Error	Set	Y(Exp)	Y(Pred)	Error
YZ22 [47]	train	22.4	20.6734	-1.727	train	1.10	1.0723	-0.0277	train	25.1	24.5351	-0.565
SFDT-TMD [48]	test	21.7	19.0695	-2.630	train	1.13	1.0846	-0.0454	train	24.1	23.6637	-0.436
MeOTTVT [49]	train	21.3	19.6635	-1.636	test	1.11	1.0536	-0.0564	train	23.89	23.642	-0.248
DTP-C6Th [50]	train	21.04	21.1295	0.089	test	1.15	1.1143	-0.0357	test	22.76	22.9099	0.149
TQ4 [51]	train	21	18.8612	-2.139	train	1.12	1.0632	-0.0568	train	23.71	22.743	-0.967
Cz-As [52]	train	20.9	18.7362	-2.164	train	1.08	1.0777	-0.0023	train	24.4	22.6443	-1.755
DTPC13-ThTPA [53]	test	20.38	20.0375	-0.342	train	1.13	1.1264	-0.0036	train	22.82	22.9424	0.122
TTE-2 [54]	train	20.04	21.5815	1.541	train	1.11	1.1377	0.0277	train	23.26	24.0227	0.762
ZT-H2 [55]	test	19.6	18.2612	-1.339	train	1.11	1.1276	0.0176	test	24.15	23.6662	-0.484
CuPc [56]	train	19.6	19.3444	-0.256	test	1.10	1.082	-0.018	train	23.96	24.2379	0.278
H2Pc [56]	train	19.6	19.2109	-0.389	train	1.11	1.0845	-0.0255	train	23.85	24.1973	0.347
WH-1 [57]	train	19.5	19.1644	-0.336	train	1.08	1.0747	-0.0053	train	23.37	23.5002	0.130
YN2 [58]	train	19.27	17.8935	-1.376	train	1.11	1.0868	-0.0232	train	22.87	22.5398	-0.330
WH-3 [59]	train	19.2	18.28	-0.920	train	1.07	1.0437	-0.0263	test	23.05	22.8557	-0.194
tpa-t-FBTD [60]	train	18.9	18.6796	-0.220	train	1.08	1.0709	-0.0091	train	22.4	22.3783	-0.022
FA-CN [61]	train	18.9	18.605	-0.295	train	1.13	1.1346	0.0046	test	21.71	21.9536	0.244
Y6-T [62]	train	18.8	20.4046	1.605	train	1.10	1.1431	0.0431	train	22.9	23.458	0.56
Cz-Py [52]	train	18.2	18.7076	0.508	train	1.13	1.0944	-0.0356	train	21.9	22.4128	0.513
YZ18 [47]	test	18.1	18.3932	0.293	train	1.03	1.0382	0.0082	train	24.1	23.7412	-0.359
C202 [63]	train	17.7	18.102	0.402	test	1.05	1.0558	0.0058	train	23	23.0689	0.069
α, β-COTh-Ph-OMeTAD [64]	train	17.2	20.5569	3.357	train	1.05	1.1094	0.0594	train	21.51	22.9305	1.421
C302 [65]	train	16.4	16.0269	-0.373	train	1.01	1.0011	-0.0089	train	23.3	23.1884	-0.112
PhCz-4MeOTPA [66]	train	16	17.1082	1.108	train	1.08	1.0748	-0.0052	train	21.52	22.1857	0.666
X62 [67]	test	15.9	18.4159	2.516	train	1.01	1.0358	0.0258	train	22.4	22.7265	0.326
Spiro-IA [68]	train	15.7	14.1299	-1.570	test	1.04	0.9994	-0.0406	train	22.14	21.2679	-0.872
WH-2 [59]	train	15.3	17.3873	2.087	train	1.02	1.0357	0.0157	train	21.95	22.5337	0.584
DBT(QT-TPA)$_2$ [68]	test	13.6	14.9193	1.319	train	1.04	1.0404	0.0004	test	19.23	20.4922	1.262
T(EDOT-TPA)$_2$ [69]	train	12.3	13.7034	1.403	train	1.04	1.061	0.021	train	20.25	20.3086	0.059
TQ3 [51]	train	10.8	10.2275	-0.572	test	0.95	0.9526	0.0026	train	20.9	19.747	-1.15
ZT-H1 [55]	train	10	10.3588	0.359	train	1.00	1.0044	0.0044	test	21.21	22.2224	1.012
DT-BT [70]	train	7.3	9.9204	2.620	train	0.83	0.8922	0.0622	train	16.8	18.2419	1.442
C301 [65]	train	5.8	4.6935	-1.106	train	0.73	0.7146	-0.0154	train	19.6	19.142	-0.458

Table (S10): Experimental and predicted PCE, V_{OC}, and J_{SC} values for the test and train sets for dopant-free HTMs when used in inverted p-i-n PSCs based on mixed CLHs.

HTM	PCE				V_{OC}				J_{SC}			
	Set	Y(Exp)	Y(Pred)	Error	Set	Y(Exp)	Y(Pred)	Error	Set	Y(Exp)	Y(Pred)	Error
TPADPP [71]	train	21.6	19.1459	-2.454	train	1.12	1.0789	-0.0411	train	23.72	22.8498	-0.870
MCz-cz-BTI [72]	test	21.3	20.5839	-0.716	train	1.1	1.1201	0.0201	train	23.24	23.4828	0.243
BTORCNA [73]	train	21.1	21.0862	-0.014	train	1.1	1.0994	-0.0006	train	22.84	22.423	-0.417
MPA-CZ-PTI [72]	train	20.8	20.2339	-0.566	test	1.07	1.0797	0.0097	test	22.84	22.7844	-0.056

HTM-F [74]	train	20.5	19.1836	-1.316	train	1.09	1.0374	-0.0526	train	23.03	22.7339	-0.296
N01 [75]	train	20.4	21.1483	0.748	train	1.08	1.0968	0.0168	test	23.65	23.856	0.206
BTF6 [76]	train	20.3	16.5064	-3.794	train	1.13	1.0009	-0.1291	train	22.23	21.7526	-0.477
TPA-FO [77]	train	20.2	18.8534	-1.347	train	1.09	1.0819	-0.0081	train	22.76	21.8814	-0.879
BTORA [73]	test	20.2	20.4188	0.219	test	1.09	1.0853	-0.0047	train	22.1	22.4439	0.344
MCZ-PA-PTI [72]	train	20	19.869	-0.131	train	1.08	1.0634	-0.0166	train	22.66	23.0055	0.345
HTM-H [78]	train	19	19.2417	0.242	train	1.05	1.04	-0.01	train	22.7	22.4097	-0.290
N02 [75]	train	18.9	20.9026	2.003	train	1.03	1.0875	0.0575	train	23.48	23.856	0.376
BTRA [73]	test	18.4	19.3275	0.927	test	1.06	1.0572	-0.0028	train	21.64	22.1964	0.556
MPA-PA-BTI [72]	train	17.4	18.8626	1.463	train	0.99	1.0182	0.0282	test	22.15	22.6347	0.485
TPA-PDO [77]	train	17	18.2141	1.214	train	1.03	1.0733	0.0433	train	20.44	21.2302	0.790
TPADPP-Boc [71]	train	16.3	18.2774	1.977	train	1.02	1.0602	0.0402	train	22.22	22.4288	0.209
BTF5 [76]	train	11.4	13.3748	1.975	train	0.8	0.8519	0.0519	train	21.31	21.6758	0.366

Overview of the AutoQSAR Methodology

The AutoQSAR workflow is outlined in **Figure 3** in the manuscript. In this workflow, a subset of descriptors is independently applied to various machine learning methods, including Kernel Partial Least Squares (KPLS), Partial Least Squares (PLS), Multiple Linear Regression (MLR), and Principal Component Regression (PCR). These models are trained using continuous independent variables, which is the focus of this study.

Number of Models to Build for Each Model Type: AutoQSAR enables users to specify the number of models to construct for each model type. A model is defined by randomly selecting training and test sets based on the percentage split specified in the AutoQSAR panel. Each training set is utilized to build models using all supported machine learning methods (KPLS, PLS, MLR, and PCR) alongside relevant combinations of independent variables (e.g., descriptors). In this study, the AutoQSAR panel was used to develop a total of 50 models, **Figure S1**. The performance of each model is evaluated based on its predictive ability on the test set, resulting in a quality score for each model. Model accuracy is scored on a scale from 0 to 1, where a score of 1 represents perfect predictions and a score of 0 indicates entirely incorrect predictions.

Top Models and Predictions: AutoQSAR can identify the top models for further predictions. In this study, we retained the top 10 ranked models. Predictions can be made using either individual models or a consensus of the top 10 models. For continuously valued dependent variables, the consensus prediction is calculated as the arithmetic mean of the predictions from the selected models, see **Figure S1**.

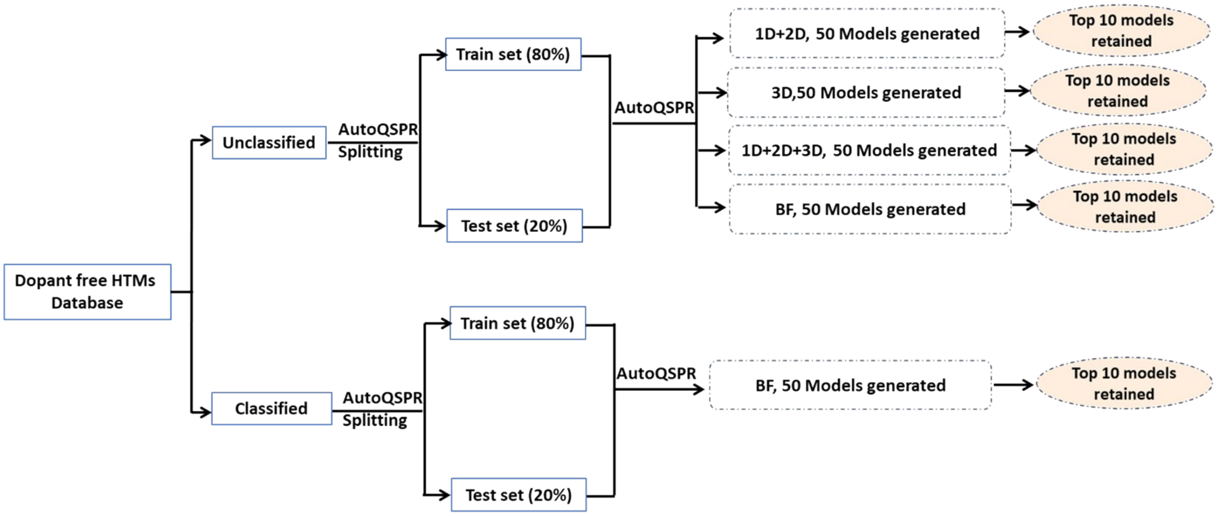
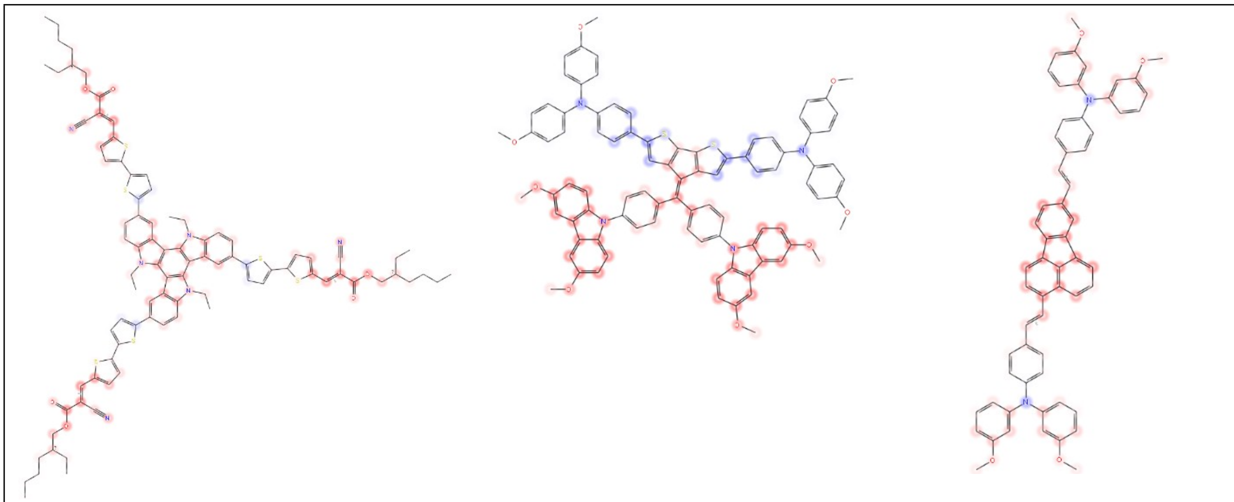


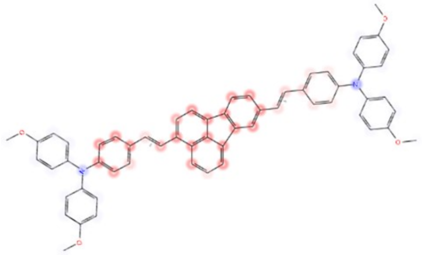
Fig. S1. Strategy used for building QSPR models with the assistance of AutoQSPR. The top-ranked models were selected based on their ranking scores. BF refers to binary fingerprints.

Model Visualization

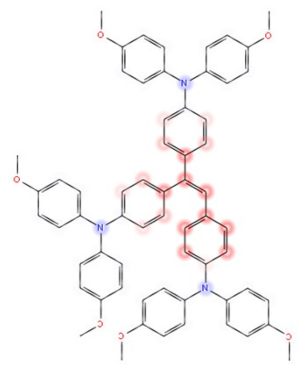
1- Visualizing Conventional (n-i-p) PSCs based on MALX$_3$ for PCE



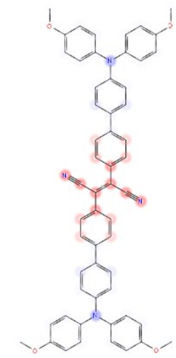
TAT–2T–CAN	**C-CPDT**	**FBA3**
Obs: 20.10	Obs: 19.60	Obs: 19.27
Pred: 20.48	Pred: 19.27	Pred: 19.49



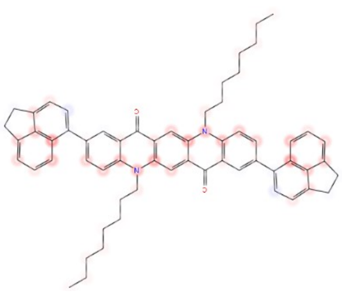
FBA2
Obs: 18.70
Pred: 19.00



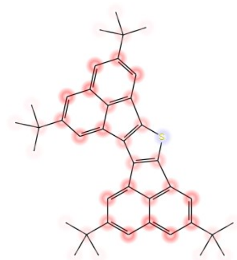
CJ-01
Obs: 18.56
Pred: 18.08



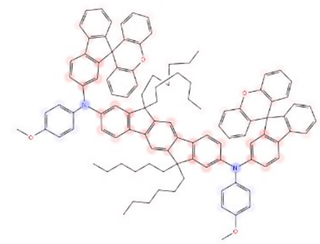
TPA–BPFN–TPA
Obs: 18.40
Pred: 17.90



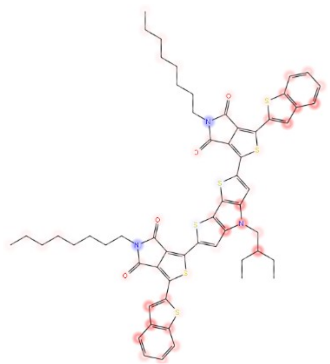
ACE-QA-ACE
Obs: 18.20
Pred: 17.30



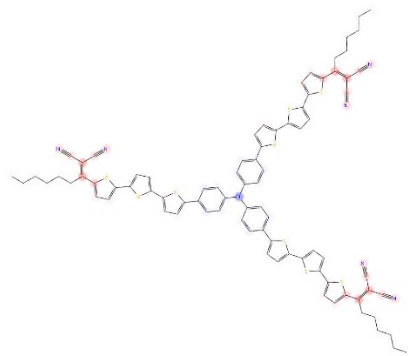
PCA-1
Obs: 18.17
Pred: 18.24



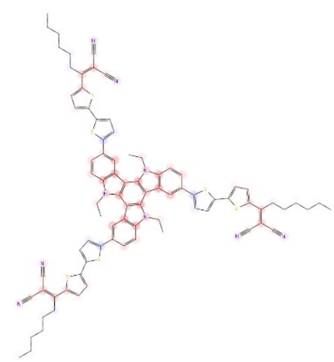
IDF-SFXPh
Obs: 17.60
Pred: 17.38



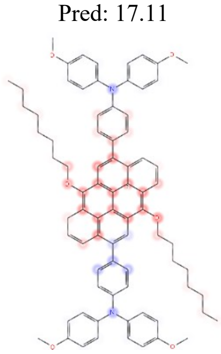
BTDTP
Obs: 17.60
Pred: 17.11



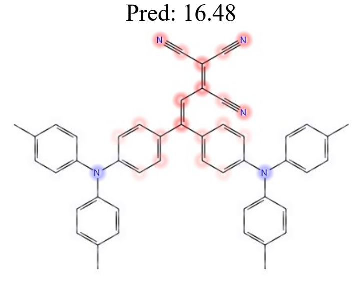
TPA–3T–DCV
Obs: 17.60
Pred: 16.48



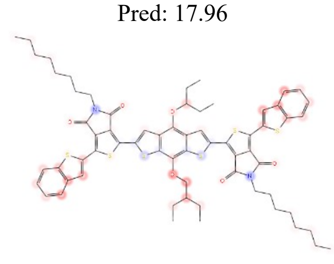
TPA–2T–DCV
Obs: 17.60
Pred: 17.96



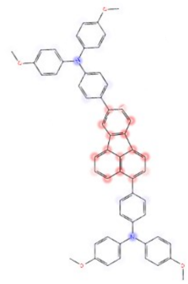
TPA-ANT-TPA
Obs: 17.50
Pred: 17.55



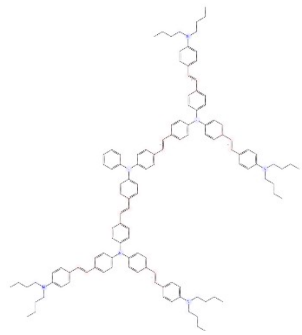
BTPA-TCNE
Obs: 16.94
Pred: 17.30



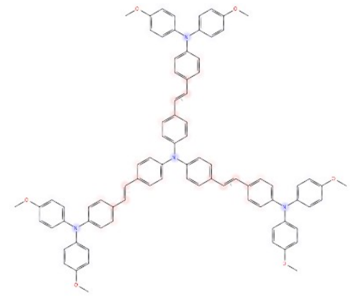
BTBDT
Obs: 16.90
Pred: 16.76



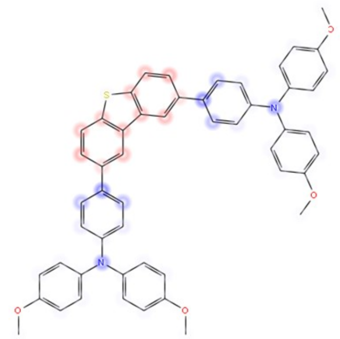
FBA1
Obs: 16.80
Pred: 16.52



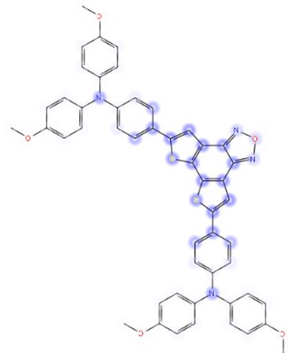
Z1011
Obs: 16.30
Pred: 16.09



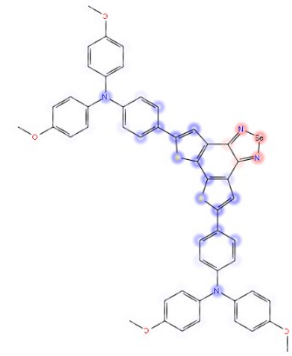
Z34
Obs: 16.10
Pred: 16.39



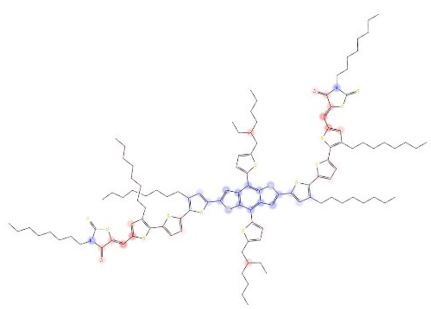
CQ2
Obs: 15.20
Pred: 14.77



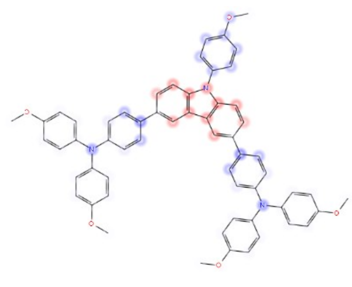
DTBT
Obs: 11.60
Pred: 12.12



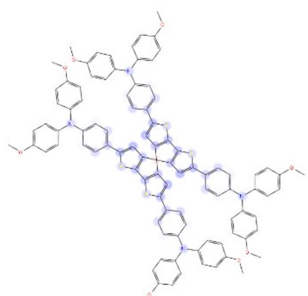
DTBS
Obs: 15.00
Pred: 13.08



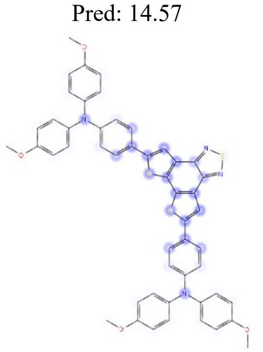
DOR3T-TBDT
Obs: 14.90
Pred: 14.57



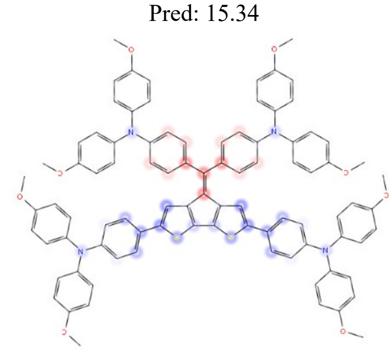
X25
Obs: 14.40
Pred: 15.34



HTM1
Obs: 13.40
Pred: 12.97



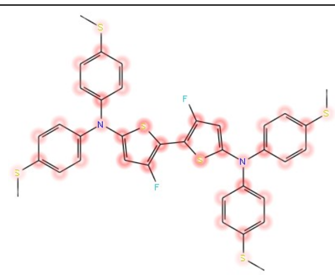
DTBF
Obs: 13.30
Pred: 12.63



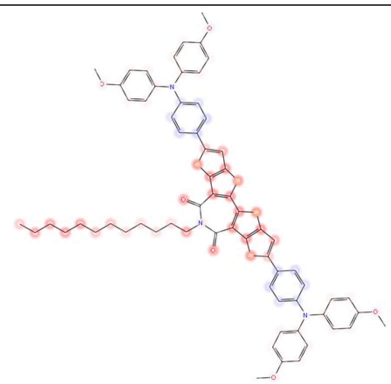
T-CPDT
Obs: 11.40
Pred: 14.23

Figure S2. Visualization of atomic effects for KPLS model built for the power conversion efficiency from dendritic fingerprints for dopant free HTMs used in conventional (n-i-p) PSCs based on $MAPbX_3$. Prediction of Marcus theory reorganization energies *are* shown with positive or negative site contributions shown as red and blue, respectively.

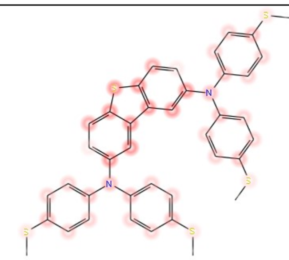
2- Visualizing Inverted (p-i-n) PSCs based on $MAPbX_3$ for PCE



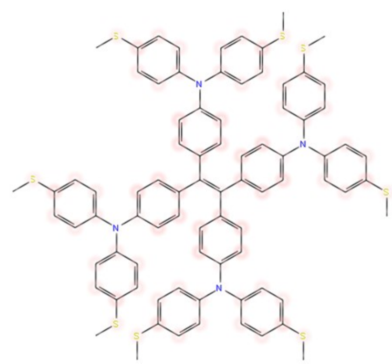
DFBT-MTP
Obs: 21.2
Pred: 21.5444



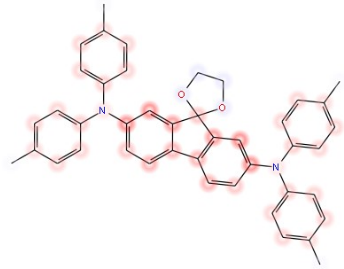
MPA-BTTI
Obs: 21.17
Pred: 21.01



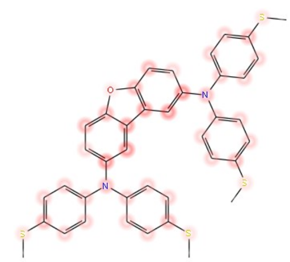
DBTMT
Obs: 21.10
Pred: 22.45



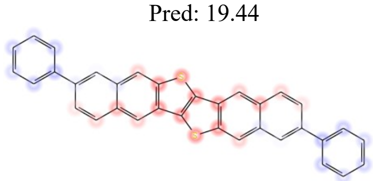
TPE-S
Obs: 21.00
Pred: 19.44



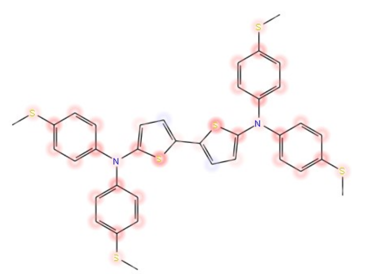
DFH
Obs: 20.60
Pred: 20.05



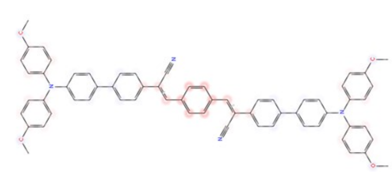
DBFMT
Obs: 20.50
Pred: 20.75



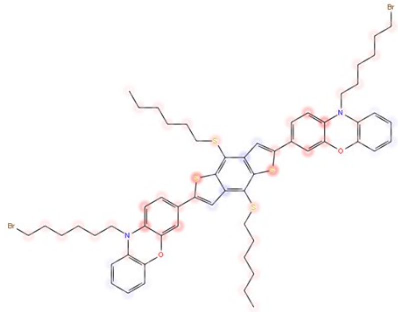
DPh-DNTT
Obs: 20.10
Pred: 19.22



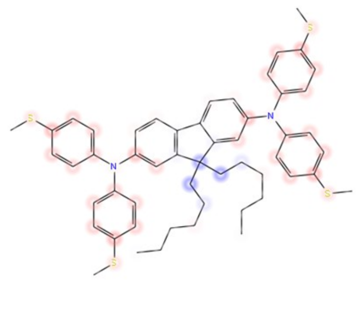
BT-MTP
Obs: 20.10
Pred: 19.86



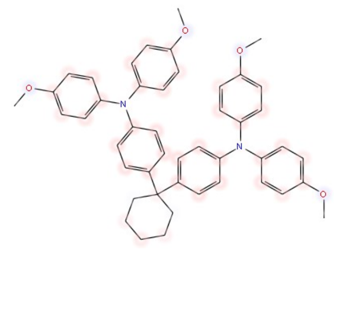
YJ01
Obs: 19.80
Pred: 18.20



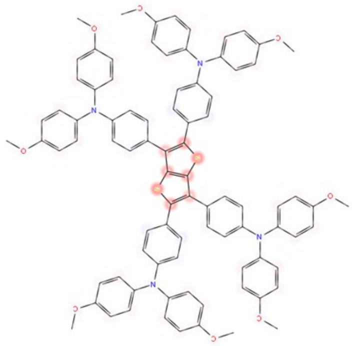
BDT-POZ
Obs: 19.16
Pred: 19.13



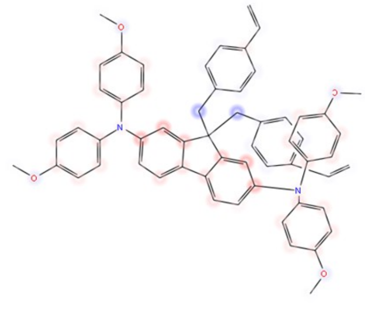
FMT
Obs: 19.06
Pred: 19.58



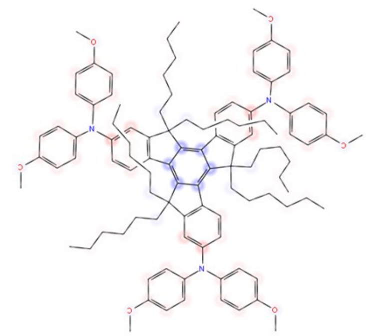
TAPC
Obs: 18.80
Pred: 18.57



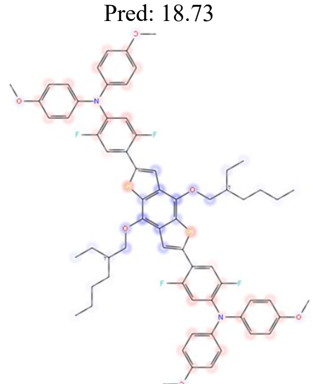
XY1
Obs: 18.78
Pred: 18.73



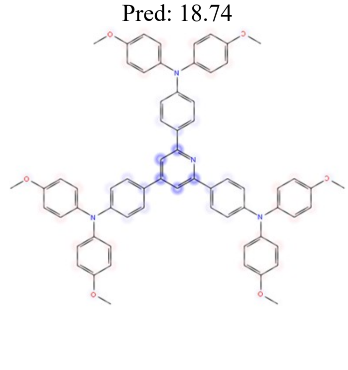
VB-MeO-FDPA
Obs: 18.70
Pred: 18.74



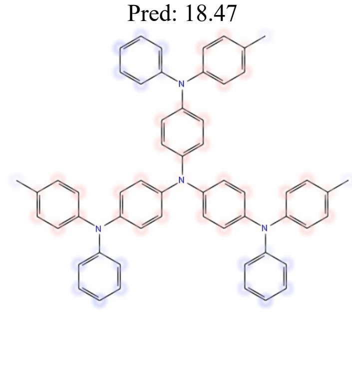
Trux-OMeTAD
Obs: 18.60
Pred: 18.47



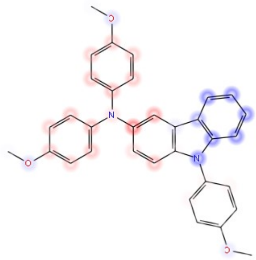
H2
Obs: 18.60
Pred: 18.90



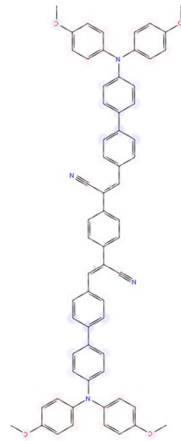
D106
Obs: 18.20
Pred: 17.07



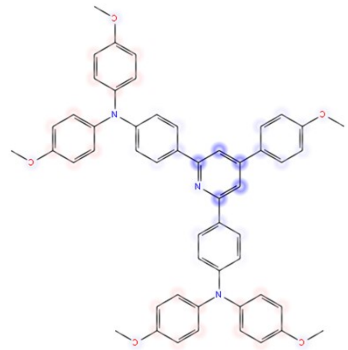
m-MTDATA
Obs: 18.12
Pred: 18.05



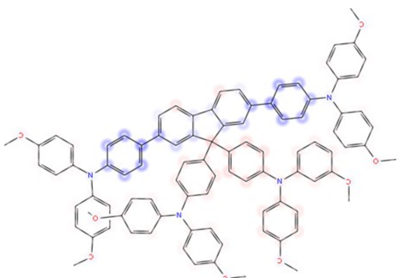
TPAC3M
Obs: 17.54
Pred: 17.64



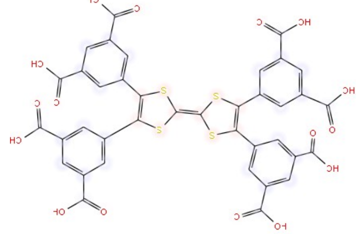
YJ02
Obs: 17.50
Pred: 17.37



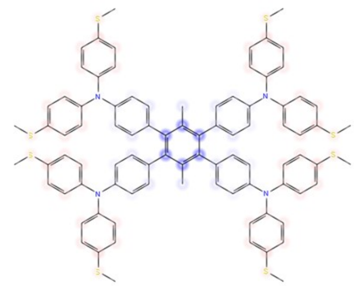
D105
Obs: 17.40
Pred: 17.07



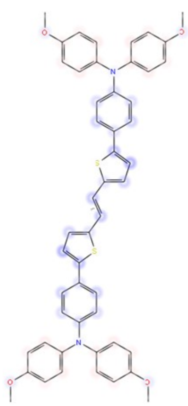
TPA-2,7-FLTPA-TPA
Obs: 17.10
Pred: 17.11



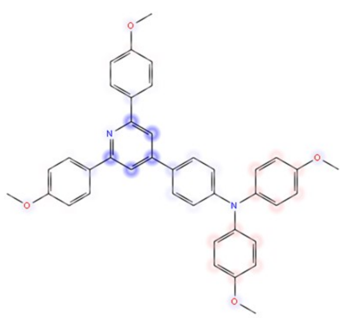
TTA
Obs: 16.70
Pred: 17.22



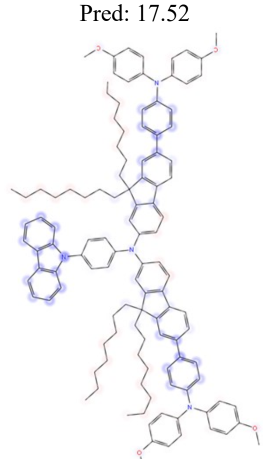
TPP-SMeTAD
Obs: 16.60
Pred: 17.52



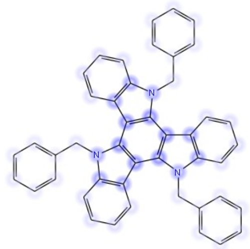
TPA-TVT-TPA
Obs: 16.32
Pred: 17.00



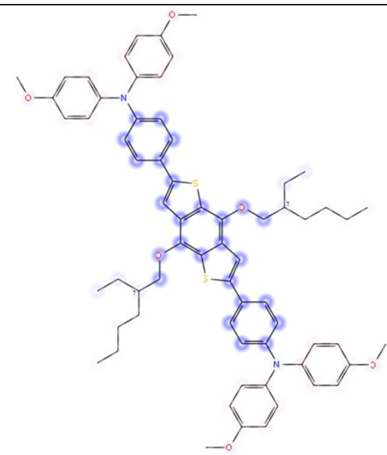
D104
Obs: 16.20
Pred: 17.07



CzPAF-TPA
Obs: 15.71
Pred: 15.34



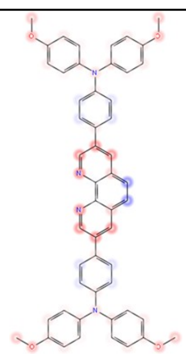
TBDI
Obs: 15.33
Pred: 14.85



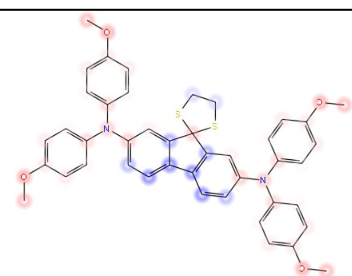
H0
Obs: 13.30
Pred: 14.74

Figure S3. Visualization of atomic effects for KPLS model built for the power conversion efficiency from linear fingerprints for dopant free HTMs used in inverted (p-i-n) PSCs based on $MAPbX_3$. Prediction of Marcus theory reorganization energies *are* shown with positive or negative site contributions shown as red and blue, respectively.

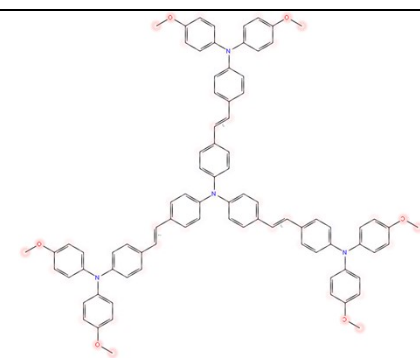
3- Visualizing Conventional (n-i-p) PSCs based on mixed cation lead halide for PCE.



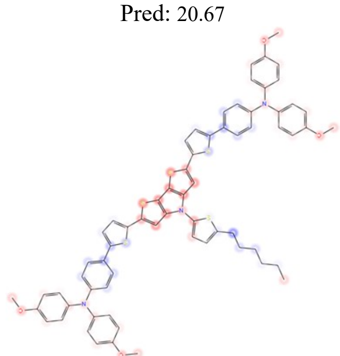
YZ22
Obs: 22.4
Pred: 20.67



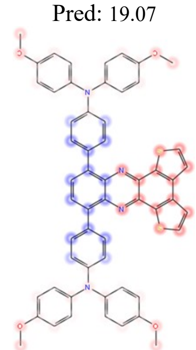
SFDT-TMD
Obs: 21.7
Pred: 19.07



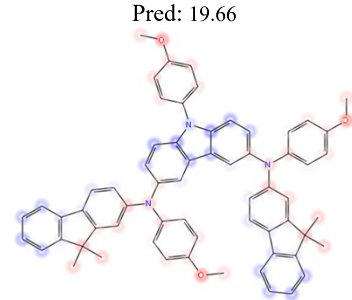
MeOTTVT
Obs: 21.3
Pred: 19.66



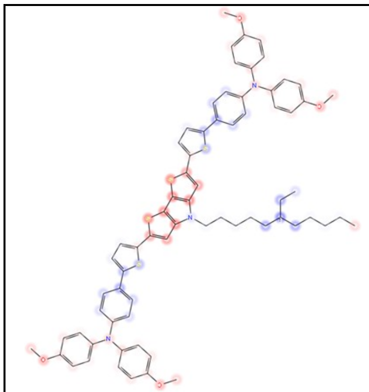
DTP-C6Th
Obs: 21.04
Pred: 21.13



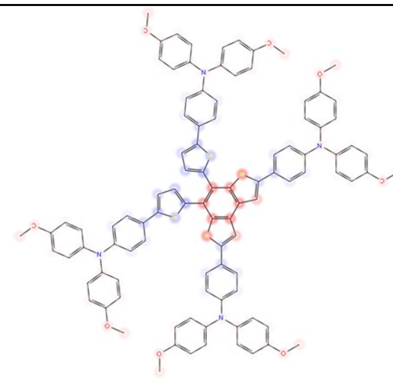
TQ4
Obs: 21.00
Pred: 18.86



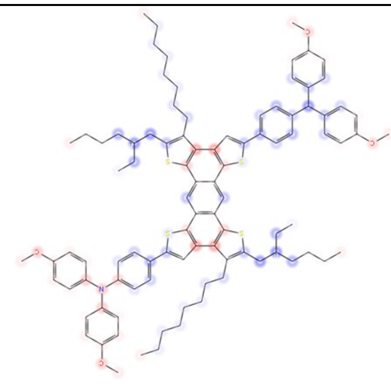
Cz-As
Obs: 20.90
Pred: 18.74



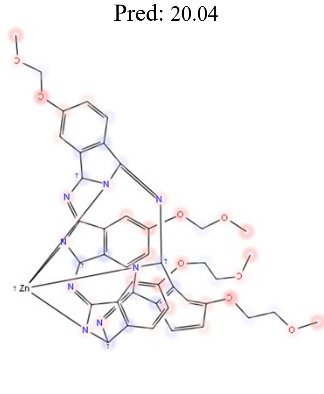
DTPC13-ThTPA
Obs: 20.38
Pred: 20.04



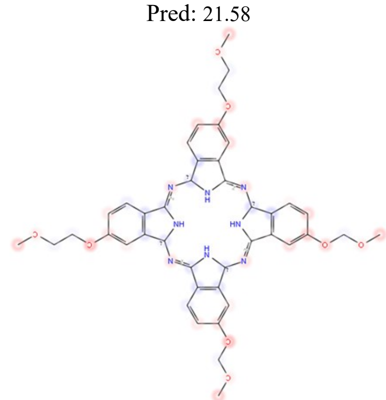
TTE-2
Obs: 20.04
Pred: 21.58



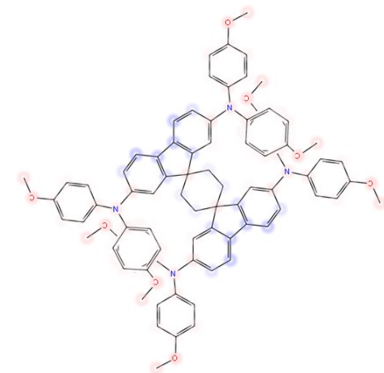
ZT-H2
Obs: 19.60
Pred: 18.26



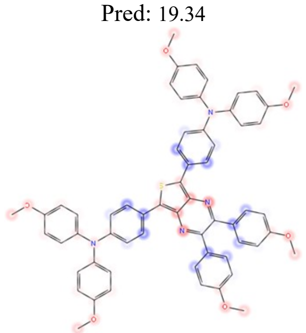
CuPc
Obs: 19.60
Pred: 19.34



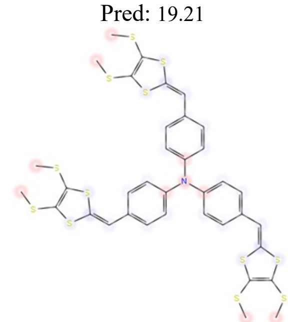
H2Pc
Obs: 19.60
Pred: 19.21



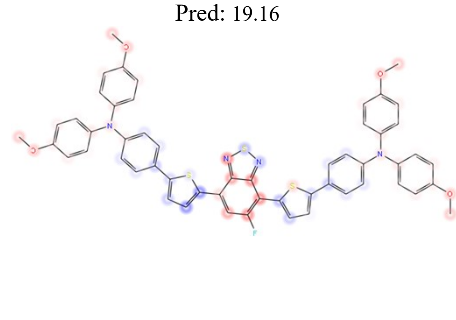
WH-1
Obs: 19.50
Pred: 19.16



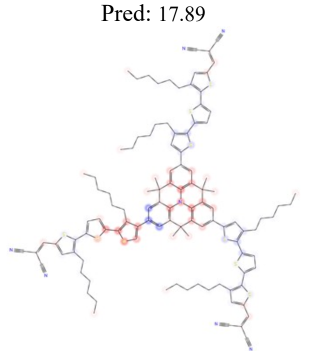
YN2
Obs: 19.27
Pred: 17.89



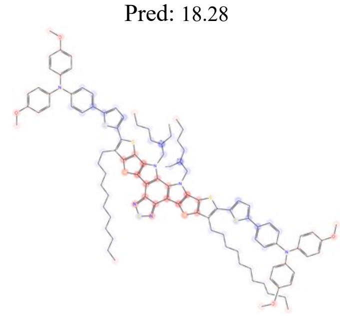
WH-3
Obs: 19.20
Pred: 18.28



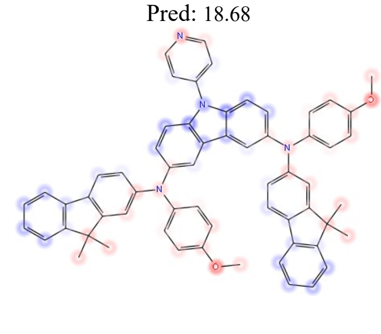
tpa-t-FBTD
Obs: 18.90
Pred: 18.68



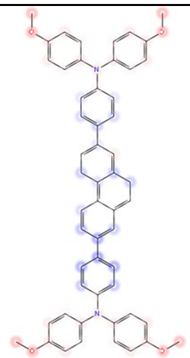
FA-CN
Obs: 18.90
Pred: 18.60



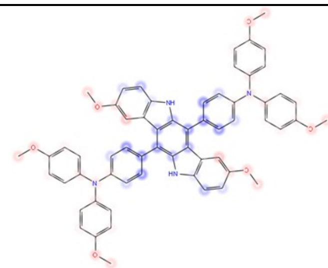
Y6-T
Obs: 18.80
Pred: 20.40



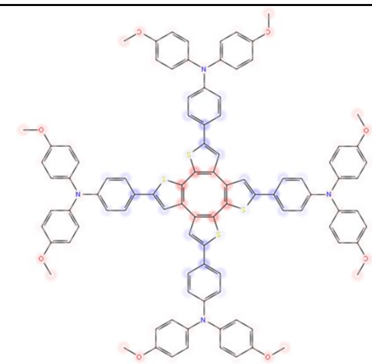
Cz-Py
Obs: 18.20
Pred: 18.71



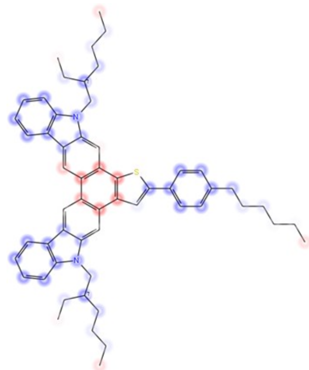
YZ18
Obs: 18.10
Pred: 18.39



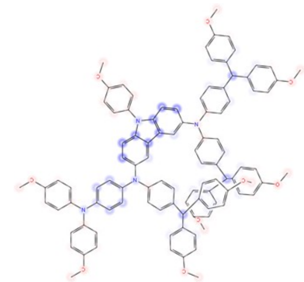
C202
Obs: 17.70
Pred: 18.10



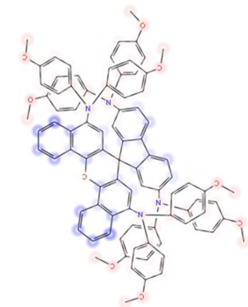
α, β-COTh-Ph-OMeTAD
Obs: 17.20
Pred: 20.56



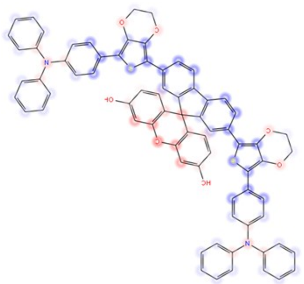
C302
Obs: 16.40
Pred: 16.03



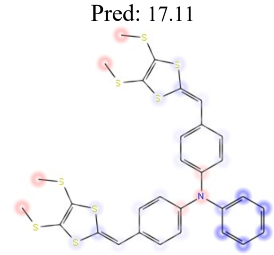
PhCz-4MeOTPA
Obs: 16.00
Pred: 17.11



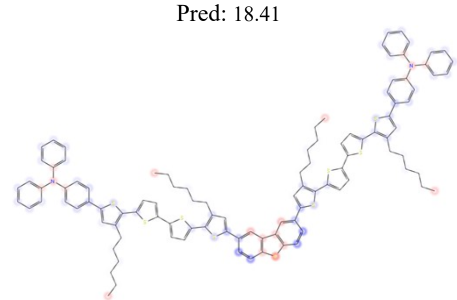
X62
Obs: 15.90
Pred: 18.41



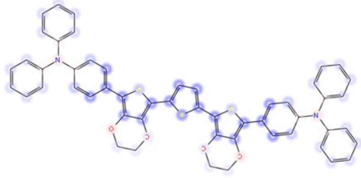
Spiro-IA
Obs: 15.70
Pred: 14.13



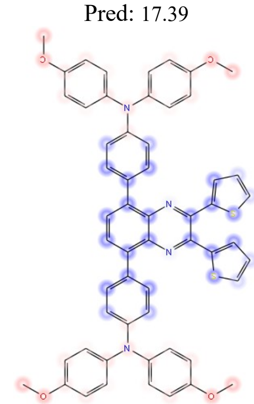
WH-2
Obs: 15.30
Pred: 17.39



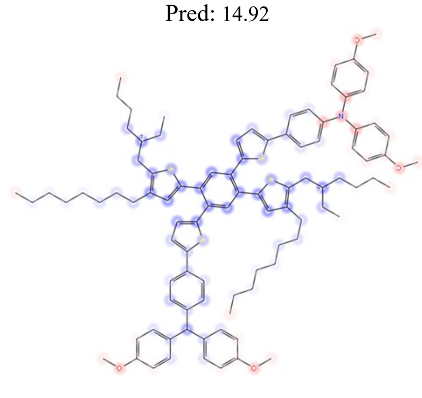
DBT(QT-TPA)$_2$
Obs: 13.60
Pred: 14.92



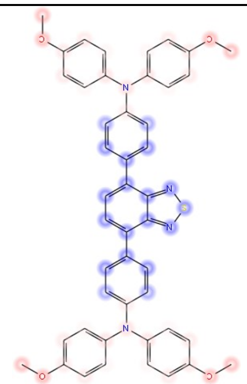
T(EDOT-TPA)$_2$
Obs: 12.30
Pred: 13.70



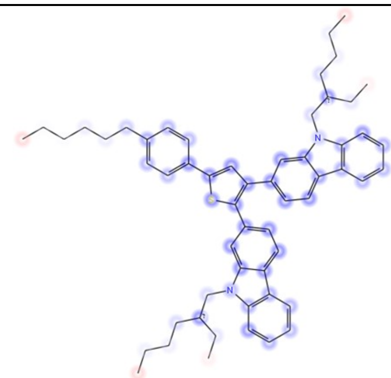
TQ3
Obs: 10.80
Pred: 10.23



ZT-H1
Obs: 10.00
Pred: 10.36



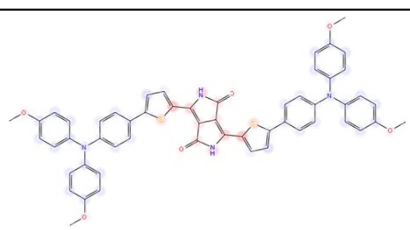
DT-BT
Obs: 7.30
Pred: 9.92



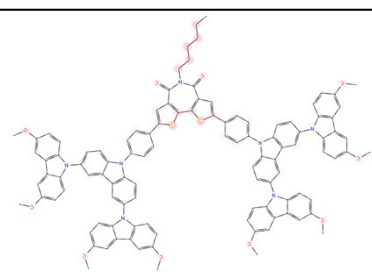
C301
Obs: 5.80
Pred: 4.69

Figure S4. Visualization of atomic effects for KPLS model built for the power conversion efficiency from dendritic fingerprints for dopant free HTMs used in conventional (n-i-p) PSCs based on mixed cation lead halide. Prediction of Marcus theory reorganization energies are shown with positive or negative site contributions shown as red and blue, respectively.

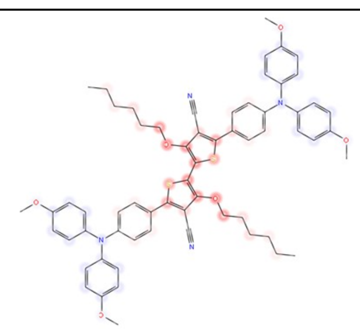
4- Visualizing Inverted (p-i-n) PSCs based on mixed cation lead halide for PCE.



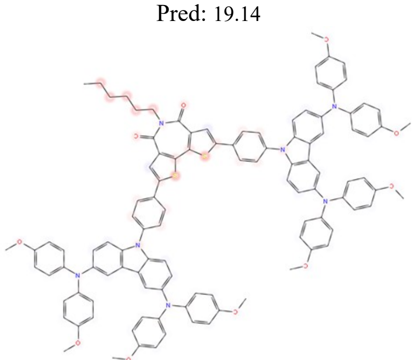
TPADPP
Obs: 21.60
Pred: 19.14



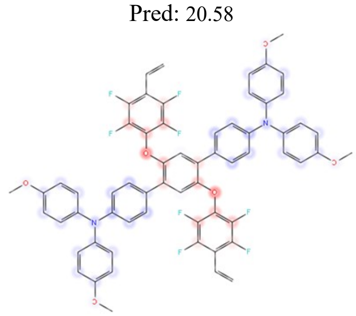
MCz-cz-BTI
Obs: 21.30
Pred: 20.58



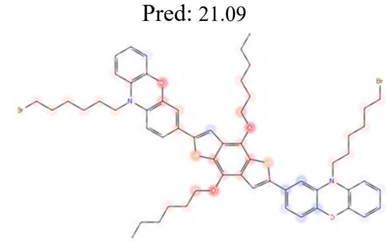
BTORCNA
Obs: 21.10
Pred: 21.09



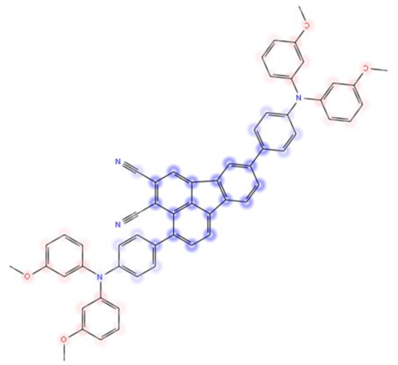
MPA-CZ-PTI
Obs: 20.80
Pred: 20.23



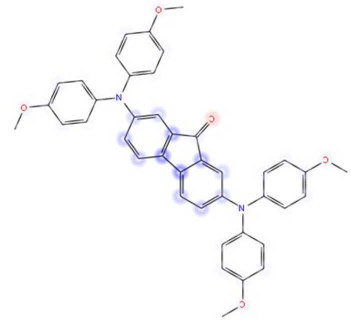
HTM-F
Obs: 20.50
Pred: 19.18



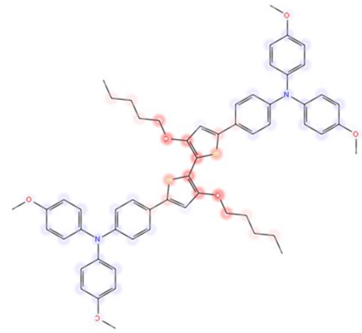
N01
Obs: 20.40
Pred: 21.15



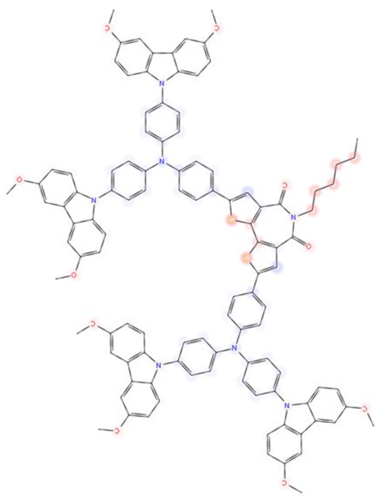
BTF6
Obs: 20.30
Pred: 16.51



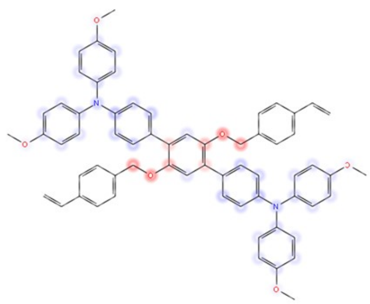
TPA-FO
Obs: 20.20
Pred: 18.85



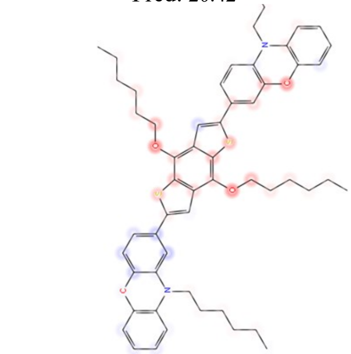
BTORA
Obs: 20.20
Pred: 20.42



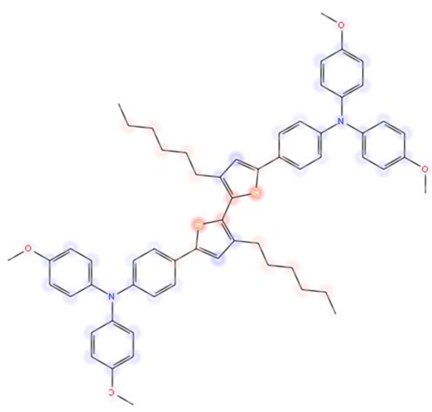
MCZ-PA-PTI
Obs: 20.00
Pred: 19.87



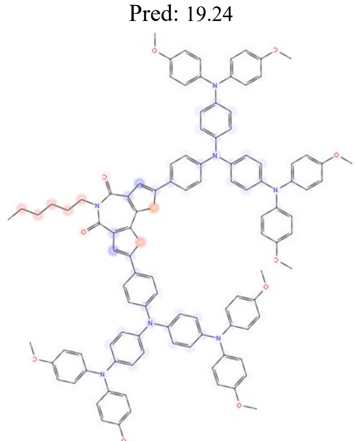
HTM-H
Obs: 19.00
Pred: 19.24



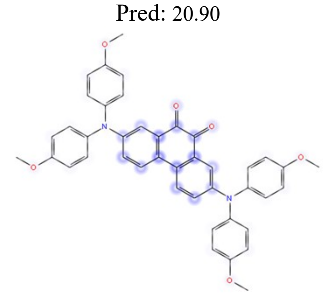
N02
Obs: 18.90
Pred: 20.90



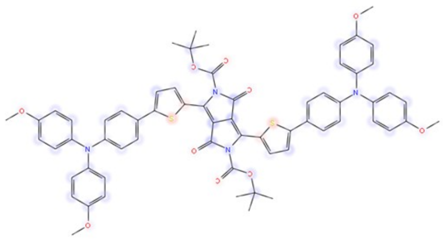
BTRA
Obs: 18.40
Pred: 19.33



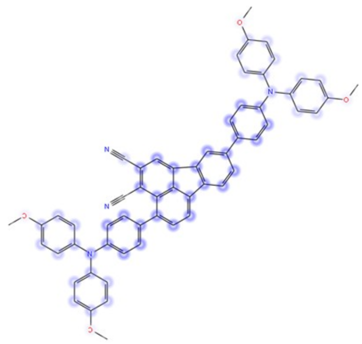
MPA-PA-BTI
Obs: 17.40
Pred: 18.86



TPA-PDO
Obs: 17.00
Pred: 18.21



TPADPP-Boc
Obs: 16.30
Pred: 18.28



BTF5
Obs: 11.40
Pred: 13.37

Figure S5. Visualization of atomic effects for KPLS model built for the power conversion efficiency from linear fingerprints for dopant free HTMs used in inverted (p-i-n) PSCs based on mixed cation lead halide. Prediction of Marcus theory reorganization energies *are* shown with positive or negative site contributions shown as red and blue, respectively.

Table (S11). Experimental and predicted photovoltaic properties of the fabricated PSCs based on dopant-free HTMs for external model validation.

Conventional PSCs based on $MAPbX_3$ Perovskite										
HTM	**PCE^{ex}**	**PCE^{AP}**	**PCE^{CP}**	**J_{SC}^{ex}**	**J_{SC}^{AP}**	**J_{SC}^{CP}**	**V_{OC}^{ex}**	**V_{OC}^{AP}**	**V_{OC}^{CP}**	**Ref**
CB	20.76	16.802	16.59	23.72	22.386	22.14	1.15	1.032	1.06	[79]
DERDTS-TBDT	16.2	16.873	15.86	21.2	22.061	21.78	1.05	1.044	0.99	[80]
ST1	15.4	18.675	16.77	21.07	22.296	20.91	1.059	1.094	1.08	[81]
mDPA-DBTP	18.9	19.232	16.31	21.1	22.91	22.60	1.12	1.082	1.02	[82]
TPA-BPFN-TPA	18.4	18.165	17.85	22.7	22.251	21.87	1.04	1.041	1.033	[83]
Inverted PSCs based on $MAPbX_3$ Perovskite										
TTA	16.7	17.84	18.32	20.4	21.413	20.88	1.04	1.054	1.071	[84]
TM-2	16.13	19.044	18.70	20.08	22.562	22.55	1.04	1.072	1.040	[85]
TM-3	15.78	18.91	18.82	20.27	22.571	22.58	1.01	1.07	1.046	[85]
YJS001	17.02	15.639	17.28	21.97	21.557	21.45	1.052	1.005	1.060	[86]
YJS003	20.11	15.726	17.68	22.94	21.567	21.70	1.091	1.016	1.073	[86]
Conventional PSCs based on mixed lead halide Perovskite										
M3	15.6	17.385	17.23	20.7	23.767	22.81	1.085	1.042	1.047	[87]
TPA-CN	17.5	16.553	15.23	20.85	20.845	21.24	1.09	1.068	1.060	[88]
RSe-CF	12.4	15.307	13.75	17.37	21.532	20.78	1.10	1.021	0.996	[89]
RSe-R	15.9	15.752	14.22	21.27	21.593	21.00	1.12	1.033	1.016	[89]
CZ-TA	18.32	16.717	16.45	21.6	21.735	22.65	1.04	1.039	1.041	[90]
Inverted PSCs based on mixed lead halide Perovskite										
TFM	16.03	17.528	16.32	22.6	21.639	21.87	0.97	1.023	0.964	[91]
MPA-PA-BTI	17.41	19.099	18.71	22.1	22.708	22.65	0.99	1.037	1.004	[92]
MPA-Cz-BTI	20.81	20.509	19.90	22.8	23.165	22.74	1.07	1.074	1.062	[92]
MCz-PA-BTI	20.09	20.894	19.82	22.6	23.074	22.89	1.08	1.088	1.055	[92]
MCz-Cz-BTI	21.35	21.234	20.57	23.2	23.271	23.10	1.10	1.097	1.098	[92]

Where PCE^{ex}, J_{SC}^{ex}, and V_{OC}^{ex} are the experimental photovoltaic parameters. PCE^{AP}, J_{SC}^{AP}, and V_{OC}^{AP} are the predicted photovoltaic parameters using the models that were developed from unclassified HTMs database. PCE^{CP}, J_{SC}^{CP}, and V_{OC}^{CP} are the predicted photovoltaic parameters utilizing the models that were developed based on classified HTMs database.

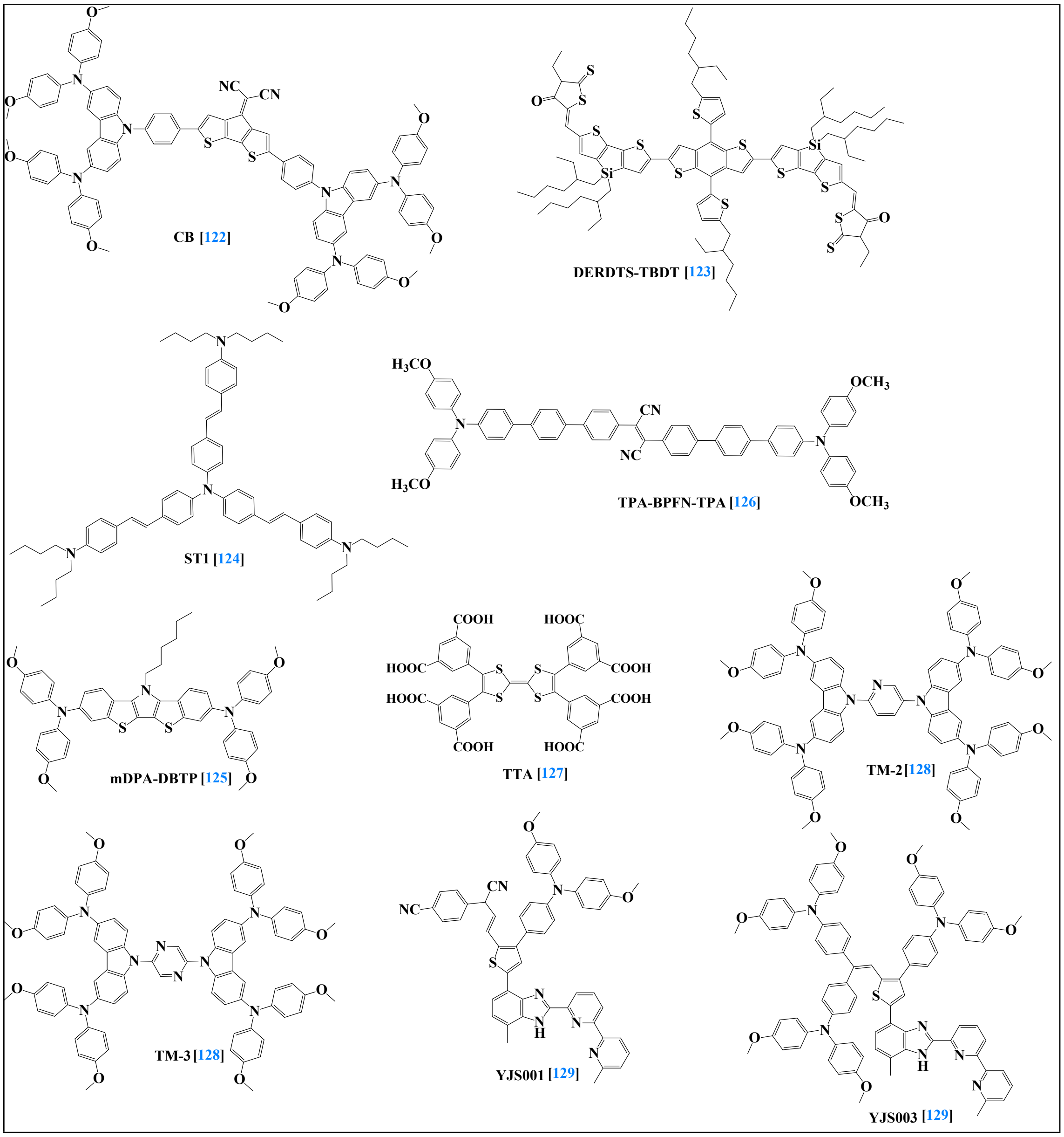


Fig. S6. Chemical Structures of the HTMs used for the validation of the ML model based on PSCs fabricated in MALHs for conventional (n-i-p) and inverted (p-i-n).

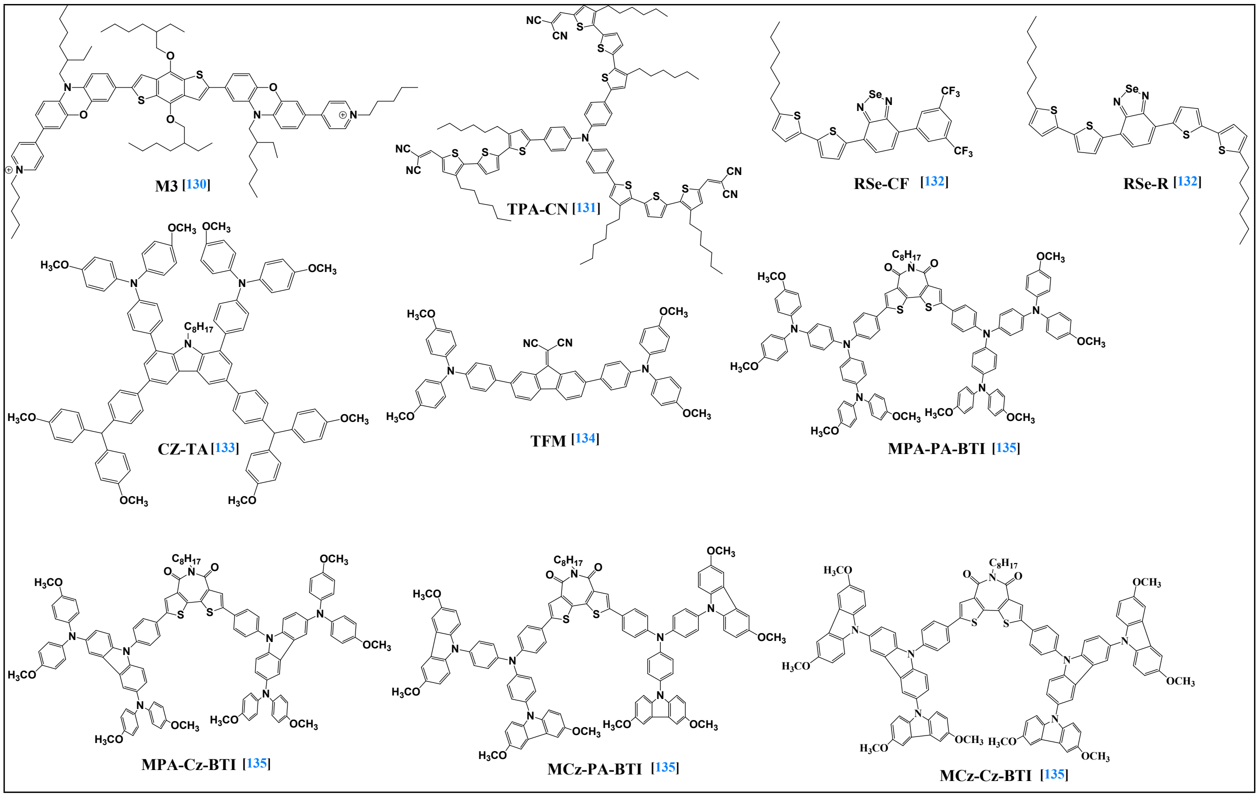


Fig. S7. Chemical structures of the HTMs utilized for the validation of ML model. This model is based on the performance of PSCs based on mixed CLHs for conventional (n-i-p) and inverted (p-i-n) devices.

List of Developed AutoQSPR Models and Calculated Molecular Descriptors in a Machine-Readable Format.

These model files can be used with the AutoQSAR tool in the Schrödinger Suite 2023-4 Release: Maestro 13.3 to apply the consensus or top-ranked QSPR models for compounds input in SMILES, 2D or 3D structure files.

1. AutoQSPR Models for HTMs Without Considering the Fabrication Method of PSCs

1.1. 3D Molecular Descriptors

- Access of the calculated 3D molecular descriptors for dopant-free HTMs along with their PSCs photovoltaic properties [here].

1.1.1. Developed autoQSPR model for the short circuit current (J_{SC}) utilizing the 3D descriptors: [link].

1.1.2. Developed autoQSPR model for the power conversion efficiency (*PCE*) utilizing the 3D descriptors: [link].

1.1.3. Developed autoQSPR model for the open circuit voltage (V_{OC}) utilizing the 3D descriptors: [link].

1.2. 1D, and 2D Molecular Descriptors

- Access the calculated 1D, and 2D molecular descriptors for dopant-free HTMs along with their photovoltaic properties [here].

1.2.1. Developed autoQSPR model for the J_{SC} utilizing 1D, and 2D descriptors: [link].

1.2.2. Developed autoQSPR model for the *PCE* utilizing 1D, and 2D descriptors: [link].

1.2.3. Developed autoQSPR model for the V_{OC} utilizing 1D, and 2D descriptors: [link].

1.3. 1D, 2D, and 3D Molecular Descriptors

- Access the calculated 1D, 2D, and 3D molecular descriptors for dopant-free HTMs along with their photovoltaic properties [here].

1.3.1. Developed autoQSPR model for the J_{SC} utilizing the 1D, 2D, and 3D descriptors: [link].

1.3.2. Developed autoQSPR model for the PCE utilizing the 1D, 2D, and 3D descriptors: [link].

1.3.3. Developed autoQSPR model for the V_{OC} utilizing the 1D, 2D, 3D descriptors: [link].

1.4. 2D Binary Fingerprints Descriptors.

- These descriptors automatically calculated using the Schrödinger suite (Schrödinger Release 2023-4: Maestro 13.3: Schrodinger LLC, New York, NY, USA) with the AutoQSPR tool.

1.4.1. Developed autoQSPR model for the J_{SC} utilizing binary fingerprints descriptors: [link].

1.4.2. Developed autoQSPR model for the *PCE* utilizing binary fingerprints descriptors: [link].

1.4.3. Developed autoQSPR model for the V_{OC} utilizing binary fingerprints descriptors: [link].

2. AutoQSPR Models for HTMs Considering the Fabrication Methods of PSCs Utilizing 2D Binary Fingerprints Descriptors

2.1. Conventional (n-i-p) PSCs Based on $MAPbX_3$

2.1.1. Developed autoQSPR model for the J_{SC}: [link].

2.1.2. Developed autoQSPR model for the PCE: [link].

2.1.3. Developed autoQSPR model for the V_{OC}: [link].

2.2. Inverted (p-i-n) PSCs Based on $MAPbX_3$

2.2.1. Developed autoQSPR model for the J_{SC}: [link].

2.2.2. Developed autoQSPR model for the PCE: [link].

2.2.3. Developed autoQSPR model for the V_{OC}: [link].

2.3. Conventional (n-i-p) PSCs Based on Mixed Cation Lead Halide

2.3.1. Developed autoQSPR model for the J_{SC}: [link].

2.3.2. Developed autoQSPR model for the PCE: [link].

2.3.3. Developed autoQSPR model for the V_{OC}: [link].

2.4. Inverted (p-i-n) PSCs based on mixed cation lead halide

2.4.1. Developed autoQSPR model for the J_{SC}: [link].

2.4.2. Developed autoQSPR model for the PCE: [link].

2.4.3. Developed autoQSPR model for the V_{OC}: [link].

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