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Supporting information for an Automated Quantum Chemistry-Driven Experimental Characterization for High PCE Donor-π-Acceptor NIR Molecular Dyes

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Table S1: Benchmark absorption energies for the quantum methods: CAM-B3LYP/6-311G(d,p), BHandHLYP/6-311G(d,p), PBE0/6-311G(d,p), the statistical LSF method, and experimental λ_{max} in the vacuum model

Name	CAM-B3LYP	BHandHLYP	PBE1PBE	Exp	LSF
AP11	3.20	3.18	2.73	3.29	2.91
AP14	3.16	3.15	2.68	3.11	2.88
AP16	3.20	3.16	2.39	3.23	3.06
AP17	3.28	3.24	2.46	3.27	3.14
AP25	2.30	2.27	2.02	1.88	2.07
AP3	2.15	2.12	1.69	1.91	2.02
BTD-1	2.50	2.41	1.76	2.41	2.44
C218	2.67	2.65	2.21	2.26	2.46
C258	2.42	2.35	1.89	2.71	2.29
C271	2.81	2.80	2.52	2.44	2.50
C272	2.53	2.44	1.99	2.42	2.38
D-DAHTDTT	2.59	2.51	1.99	2.83	2.46
D1	2.34	2.29	1.74	2.18	2.24
D3	2.30	2.21	1.55	2.21	2.29
DQ5	2.41	2.36	1.94	2.27	2.25
FNE32	2.04	2.02	1.76	2.08	1.84
FNE34	2.28	2.25	1.90	1.99	2.09
FNE52	2.50	2.45	1.90	2.36	2.38
HKK-BTZ4	2.30	2.24	1.70	2.30	2.22
IQ21	2.57	2.53	2.06	2.23	2.39
IQ4	2.82	2.78	2.11	2.35	2.71
IQ6	2.63	2.58	1.96	2.29	2.52
JD21	2.37	2.36	1.90	2.13	2.21
JW1	2.32	2.30	1.91	2.10	2.14
ND1	2.22	2.19	1.83	1.92	2.04
ND2	2.40	2.38	2.14	1.94	2.14
ND3	2.22	2.20	1.91	1.86	2.01
NKX-2883	2.53	2.53	2.22	2.25	2.27
NL11	2.36	2.35	1.95	2.18	2.18
NL12	2.34	2.33	1.89	2.20	2.18
NL13	2.37	2.36	2.02	2.10	2.15
NL2	2.21	2.21	1.88	2.00	2.02
NL3	2.19	2.19	1.86	1.91	2.00
NL4	2.13	2.12	1.81	1.89	1.94
NL5	2.24	2.23	1.90	1.85	2.04
NL6	2.25	2.24	1.38	2.05	2.30
NL7	2.42	2.41	2.01	2.11	2.23

NL8	2.34	2.33	1.92	1.98	2.16
R4	2.23	2.18	1.66	2.02	2.14
R6	2.11	2.05	1.62	1.97	2.00
R6	2.11	2.05	1.62	1.97	2.00
RR9	3.12	3.08	2.48	3.11	2.92
S-DAHTDTT	2.75	2.67	2.11	2.81	2.62
S3	2.23	2.19	1.65	1.98	2.15
SGT-121	2.64	2.59	1.99	2.64	2.53
SGT-129	2.96	2.85	1.95	2.91	2.96
SGT-130	2.48	2.39	1.72	2.41	2.44
SGT-136	2.32	2.23	1.65	2.34	2.27
T-DAHTDTT	2.75	2.68	2.10	2.86	2.61
TH304	2.57	2.58	2.03	2.18	2.41
TP1	2.28	2.25	1.84	2.14	2.13
TPA-T-TTAR-A	2.87	2.82	2.27	3.00	2.69
TPA-T-TTAR-T-A	2.79	2.71	2.12	3.00	2.66
TPA-TTAR-A	2.97	2.94	2.42	2.49	2.75
TTAR-15	2.74	2.69	2.24	2.49	2.54
TTAR-9	2.84	2.77	2.24	2.39	2.67
TTAR-B8	2.72	2.68	2.24	2.56	2.51
WS-55	2.40	2.34	1.97	2.22	2.22
WS-6	2.45	2.40	1.95	2.27	2.29
XY1	2.40	2.33	1.83	2.25	2.28
Y123	2.65	2.63	2.20	2.45	2.43
YZ12	2.38	2.31	1.93	2.29	2.21
YZ15	2.34	2.26	1.87	2.26	2.19
ZL003	2.49	2.44	2.03	2.39	2.31

Table S2: Benchmark absorption energies for the quantum methods: CAM-B3LYP/6-311G(d,p), BHandHLYP/6-311G(d,p), PBE0/6-311G(d,p), the statistical LSF method, and experimental λ_{max} in the tetrahydrofuran PCM model

Name	CAM-B3LYP	BHand HLYP	PBE1PBE	Exp	LSF
AP11	3.10	3.07	2.61	3.29	2.97
AP14	3.04	3.03	2.54	3.11	2.93
AP16	3.15	3.12	2.53	3.23	3.05
AP17	3.21	3.18	2.52	3.27	3.12
AP25	2.17	2.13	1.75	1.88	2.10

AP3	2.14	2.12	1.67	1.91	2.08
BTD-1	2.48	2.39	1.75	2.41	2.45
C218	2.52	2.49	2.04	2.26	2.43
C258	2.39	2.31	1.86	2.71	2.33
C271	2.67	2.66	2.37	2.44	2.54
C272	2.52	2.44	2.00	2.42	2.44
D-DAHTDTT	2.50	2.42	1.92	2.83	2.43
D1	2.25	2.19	1.62	2.18	2.21
D3	2.23	2.13	1.50	2.21	2.21
DQ5	2.34	2.28	1.83	2.27	2.27
FNE32	1.95	1.93	1.68	2.08	1.87
FNE34	2.20	2.17	1.81	1.99	2.13
FNE52	2.44	2.38	1.81	2.36	2.39
HKK-BTZ4	2.26	2.18	1.63	2.30	2.22
IQ21	2.45	2.41	1.94	2.23	2.38
IQ4	2.73	2.68	1.96	2.35	2.68
IQ6	2.56	2.50	1.85	2.29	2.52
JD21	2.34	2.32	1.87	2.13	2.26
JW1	2.22	2.20	1.76	2.10	2.15
ND1	2.08	2.06	1.72	1.92	2.00
ND2	2.26	2.23	1.97	1.94	2.15
ND3	2.06	2.03	1.72	1.86	1.98
NKX-2883	2.38	2.38	2.04	2.25	2.28
NL11	2.28	2.26	1.83	2.18	2.21
NL12	2.31	2.28	1.84	2.20	2.23
NL13	2.27	2.26	1.88	2.10	2.19
NL2	2.11	2.10	1.75	2.00	2.03
NL3	2.09	2.08	1.73	1.91	2.01
NL4	2.02	2.01	1.67	1.89	1.95
NL5	2.15	2.14	1.82	1.85	2.06
NL6	2.18	2.16	1.74	2.05	2.11
NL7	2.36	2.34	1.91	2.11	2.28
NL8	2.25	2.25	1.81	1.98	2.18
R4	2.21	2.17	1.77	2.02	2.14
R6	2.09	2.03	1.65	1.97	2.03
RR9	3.11	3.08	2.58	3.11	3.00
S-DAHTDTT	2.65	2.57	2.05	2.81	2.58
S3	2.21	2.16	1.62	1.98	2.16
SGT-121	2.56	2.51	1.94	2.64	2.50
SGT-129	2.91	2.84	1.98	2.91	2.89
SGT-130	2.51	2.43	1.79	2.41	2.47
SGT-136	2.35	2.26	1.68	2.34	2.32

T-DAHTDTT	2.66	2.59	2.08	2.86	2.58
TH304	2.43	2.43	1.87	2.18	2.36
TP1	2.27	2.23	1.81	2.14	2.19
TPA-T-TTAR-A	2.75	2.70	2.18	3.00	2.66
TPA-T-TTAR-T-A	2.69	2.62	2.08	3.00	2.62
TPA-TTAR-A	2.84	2.81	2.29	2.49	2.75
TTAR-15	2.62	2.57	2.14	2.49	2.53
TTAR-9	2.73	2.67	2.16	2.39	2.65
TTAR-B8	2.62	2.57	2.13	2.56	2.52
WS-55	2.27	2.21	1.81	2.22	2.20
WS-6	2.35	2.30	1.81	2.27	2.29
XY1	2.33	2.25	1.83	2.25	2.26
Y123	2.52	2.49	2.09	2.45	2.42
YZ12	2.30	2.23	1.85	2.29	2.23
YZ15	2.29	2.21	1.82	2.26	2.21
ZL003	2.46	2.41	2.02	2.39	2.38

Table S3: Benchmark absorption energies for the quantum methods: CAM-B3LYP/6-311G(d,p), BHandHLYP/6-311G(d,p), PBE0/6-311G(d,p), the statistical LSF method, and experimental λ_{max} in the N,N-dimethylformanide PCM model

Name	CAM-B3LYP	BHand HLYP	PBE1PBE	Exp	LSF
AP11	3.10	3.07	2.61	3.29	2.97
AP14	3.04	3.03	2.54	3.11	2.92
AP16	3.16	3.14	2.59	3.23	3.04
AP17	3.22	3.19	2.55	3.27	3.10
AP25	2.17	2.13	1.75	1.88	2.09
AP3	2.15	2.13	1.67	1.91	2.08
BTD-1	2.50	2.41	1.77	2.41	2.43
C218	2.51	2.49	2.04	2.26	2.41
C258	2.40	2.32	1.86	2.71	2.32
C271	2.66	2.65	2.36	2.44	2.53
C272	2.53	2.45	2.02	2.42	2.43
D-DAHTDTT	2.50	2.42	1.93	2.83	2.41
D1	2.26	2.20	1.62	2.18	2.19
D3	2.23	2.14	1.51	2.21	2.18
DQ5	2.34	2.28	1.83	2.27	2.25
FNE32	1.95	1.93	1.68	2.08	1.87

FNE34	2.20	2.17	1.80	1.99	2.12
FNE52	2.44	2.38	1.81	2.36	2.36
HKK-BTZ4	2.27	2.19	1.64	2.30	2.20
IQ21	2.45	2.41	1.94	2.23	2.36
IQ4	2.73	2.68	1.96	2.35	2.65
IQ6	2.57	2.51	1.84	2.29	2.49
JD21	2.34	2.32	1.88	2.13	2.25
JW1	2.22	2.19	1.74	2.10	2.13
ND1	2.08	2.05	1.73	1.92	1.99
ND2	2.25	2.22	1.96	1.94	2.15
ND3	2.05	2.02	1.71	1.86	1.96
NKX-2883	2.37	2.37	2.02	2.25	2.26
NL11	2.29	2.27	1.82	2.18	2.20
NL12	2.32	2.29	1.85	2.20	2.23
NL13	2.27	2.25	1.87	2.10	2.18
NL2	2.11	2.10	1.74	2.00	2.02
NL3	2.09	2.08	1.73	1.91	2.01
NL4	2.02	2.00	1.66	1.89	1.94
NL5	2.15	2.14	1.82	1.85	2.05
NL6	2.18	2.16	1.73	2.05	2.10
NL7	2.36	2.34	1.90	2.11	2.26
NL8	2.25	2.25	1.81	1.98	2.17
R4	2.21	2.17	1.80	2.02	2.13
R6	2.09	2.04	1.66	1.97	2.01
RR9	3.13	3.09	2.61	3.11	3.00
S-DAHTDTT	2.65	2.57	2.06	2.81	2.56
S3	2.23	2.18	1.64	1.98	2.16
SGT-121	2.57	2.52	1.96	2.64	2.48
SGT-129	2.93	2.85	2.02	2.91	2.85
SGT-130	2.53	2.45	1.82	2.41	2.46
SGT-136	2.38	2.29	1.71	2.34	2.31
T-DAHTDTT	2.65	2.59	2.09	2.86	2.56
TH304	2.43	2.43	1.86	2.18	2.34
TP1	2.27	2.24	1.82	2.14	2.19
TPA-T-TTAR-A	2.74	2.70	2.18	3.00	2.64
TPA-T-TTAR-T-A	2.69	2.62	2.09	3.00	2.60
TPA-TTAR-A	2.84	2.80	2.29	2.49	2.73
TTAR-15	2.62	2.57	2.14	2.49	2.51
TTAR-9	2.73	2.67	2.17	2.39	2.63
TTAR-B8	2.61	2.57	2.13	2.56	2.51

WS-55	2.26	2.20	1.79	2.22	2.18
WS-6	2.35	2.31	1.81	2.27	2.27
XY1	2.33	2.25	1.84	2.25	2.24
Y123	2.52	2.49	2.09	2.45	2.41
YZ12	2.31	2.24	1.86	2.29	2.22
YZ15	2.30	2.23	1.84	2.26	2.21
ZL003	2.47	2.42	2.04	2.39	2.37

Table S4: Benchmark absorption energies for the quantum methods: CAM-B3LYP/6-311G(d,p), BHandHLYP/6-311G(d,p), PBE0/6-311G(d,p), the statistical LSF method, and experimental λ_{max} in the dichloromethane PCM model

Name	CAM-B3LYP	BHand HLYP	PBE1PBE	Exp	LSF
AP11	3.09	3.07	2.61	3.29	2.96
AP14	3.04	3.02	2.54	3.11	2.91
AP16	3.15	3.12	2.54	3.23	3.03
AP17	3.21	3.18	2.52	3.27	3.10
AP25	2.17	2.13	1.75	1.88	2.09
AP3	2.14	2.12	1.67	1.91	2.08
BTD-1	2.49	2.39	1.76	2.41	2.43
C218	2.51	2.49	2.04	2.26	2.42
C258	2.39	2.31	1.86	2.71	2.32
C271	2.66	2.65	2.36	2.44	2.53
C272	2.52	2.44	2.00	2.42	2.43
D-DAHTDTT	2.50	2.41	1.92	2.83	2.42
D1	2.25	2.19	1.62	2.18	2.20
D3	2.23	2.13	1.50	2.21	2.19
DQ5	2.34	2.28	1.83	2.27	2.26
FNE32	1.95	1.93	1.67	2.08	1.86
FNE34	2.20	2.17	1.81	1.99	2.12
FNE52	2.44	2.38	1.81	2.36	2.37
HKK-BTZ4	2.26	2.18	1.63	2.30	2.21
IQ21	2.45	2.41	1.94	2.23	2.36
IQ4	2.73	2.68	1.96	2.35	2.66
IQ6	2.56	2.50	1.85	2.29	2.50
JD21	2.34	2.32	1.87	2.13	2.25
JW1	2.22	2.19	1.75	2.10	2.14
ND1	2.08	2.05	1.72	1.92	1.99
ND2	2.25	2.22	1.97	1.94	2.14
ND3	2.05	2.02	1.71	1.86	1.96
NKX-2883	2.37	2.37	2.03	2.25	2.27

NL11	2.28	2.26	1.83	2.18	2.20
NL12	2.30	2.28	1.84	2.20	2.22
NL13	2.27	2.25	1.87	2.10	2.18
NL2	2.11	2.10	1.75	2.00	2.02
NL3	2.09	2.08	1.73	1.91	2.00
NL4	2.02	2.00	1.66	1.89	1.94
NL5	2.14	2.13	1.82	1.85	2.05
NL6	2.18	2.16	1.73	2.05	2.10
NL7	2.35	2.34	1.91	2.11	2.27
NL8	2.25	2.25	1.81	1.98	2.17
R4	2.21	2.17	1.77	2.02	2.13
R6	2.09	2.03	1.65	1.97	2.02
RR9	3.11	3.08	2.58	3.11	2.99
S-DAHTDTT	2.65	2.57	2.05	2.81	2.57
S3	2.21	2.16	1.62	1.98	2.15
SGT-121	2.56	2.51	1.94	2.64	2.49
SGT-129	2.91	2.84	1.99	2.91	2.87
SGT-130	2.51	2.43	1.79	2.41	2.46
SGT-136	2.36	2.26	1.69	2.34	2.30
T-DAHTDTT	2.65	2.59	2.08	2.86	2.56
TH304	2.43	2.43	1.86	2.18	2.35
TP1	2.27	2.24	1.81	2.14	2.18
TPA-T-TTAR-A	2.75	2.70	2.18	3.00	2.65
TPA-T-TTAR-T-A	2.69	2.62	2.08	3.00	2.61
TPA-TTAR-A	2.84	2.80	2.29	2.49	2.73
TTAR-15	2.62	2.56	2.13	2.49	2.52
TTAR-9	2.73	2.66	2.16	2.39	2.63
TTAR-B8	2.61	2.57	2.13	2.56	2.51
WS-55	2.27	2.21	1.80	2.22	2.19
WS-6	2.35	2.30	1.81	2.27	2.28
XY1	2.33	2.25	1.83	2.25	2.25
Y123	2.51	2.49	2.09	2.45	2.41
YZ12	2.30	2.23	1.85	2.29	2.22
YZ15	2.28	2.21	1.82	2.26	2.20
ZL003	2.46	2.41	2.03	2.39	2.37

Table S5: The individual benchamark data points for the LSF calculated MO diagram ordered by LUMO energies

Name	HOMO	LUMO	Wavelength
AP3	-5.11	-3.26	613

JW1	-5.17	-3.27	580
NL7	-5.34	-3.29	557
Y123	-5.39	-3.32	511
TP1	-5.30	-3.37	584
C218	-5.46	-3.39	506
C271	-5.71	-3.40	498
C258	-5.21	-3.41	543
C272	-5.28	-3.51	523
IQ21	-5.45	-3.51	519
TPA-TTAR-A	-5.75	-3.51	451
NL11	-5.34	-3.53	571
NL12	-5.28	-3.54	569
IQ4	-5.55	-3.54	458
NL13	-5.38	-3.55	578
NL8	-5.40	-3.56	576
ZL003	-5.47	-3.56	539
IQ6	-5.41	-3.56	493
YZ15	-5.12	-3.56	568
TPA-T-TTAR-A	-5.65	-3.59	461
JD21	-5.93	-3.60	562
YZ12	-5.26	-3.62	561
DQ5	-5.45	-3.63	552
RR9	-6.10	-3.63	425
SGT-121	-5.41	-3.63	491
TTAR-B8	-5.65	-3.64	494
SGT-129	-5.42	-3.64	419
XY1	-5.33	-3.65	544
FNE52	-5.45	-3.65	521
TTAR-15	-5.66	-3.67	489
T-DAHTDTT	-5.53	-3.67	475
NL2	-5.35	-3.68	616
NL4	-5.29	-3.68	640
NL5	-5.39	-3.69	608
D-DAHTDTT	-5.43	-3.69	505
S-DAHTDTT	-5.56	-3.69	475
FNE34	-5.41	-3.70	594
AP14	-6.17	-3.70	431
S3	-5.14	-3.70	578
TTAR-9	-5.69	-3.71	466
ND2	-5.56	-3.71	580
NL3	-5.34	-3.71	621
WS-55	-5.49	-3.72	561

R6	-5.11	-3.72	620
TPA-T-TTAR-T-A	-5.58	-3.72	467
SGT-136	-5.16	-3.73	548
R4	-5.19	-3.74	580
ND1	-5.31	-3.76	608
NKX-2883	-5.73	-3.78	548
AP25	-5.30	-3.78	601
ND3	-5.38	-3.78	620
AP16	-6.07	-3.79	405
WS-6	-5.56	-3.79	543
BTD-1	-5.35	-3.81	508
SGT-130	-5.31	-3.83	510
TH304	-5.66	-3.88	516
AP11	-6.35	-3.88	428
FNE32	-5.40	-3.96	674
HKK-BTZ4	-5.43	-4.00	560
D3	-5.31	-4.07	543
D1	-5.50	-4.09	554
NL6	-5.58	-4.23	540

Figure S1: A molecular orbital diagram (MO) of the LSF calculated HOMO and LUMO orbital energy for the benchmark dyes that includes the trioxide/triiodide redox shuttle and TiO_2 semiconduction conduction bans.

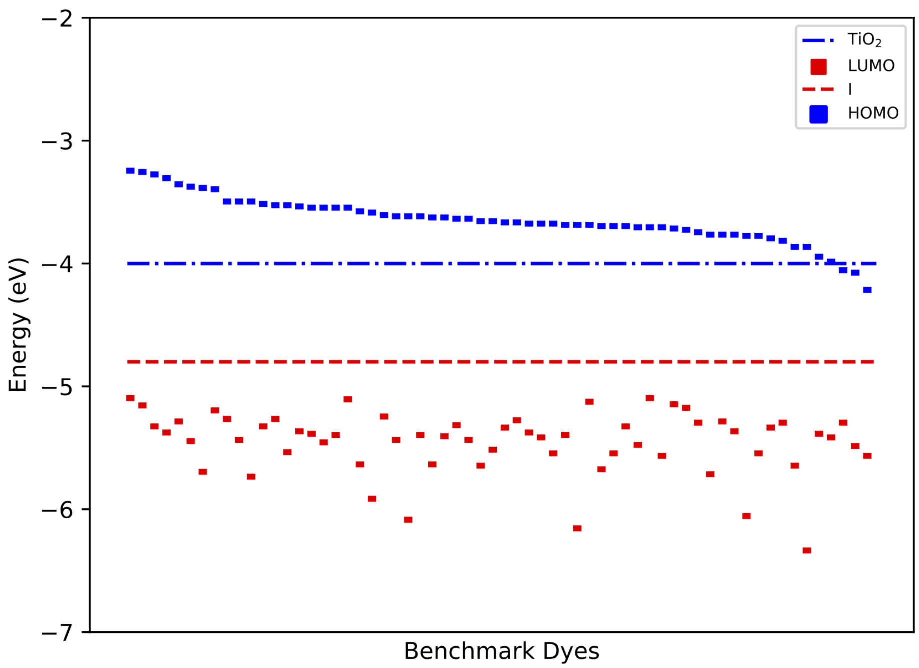


Figure S2: The benchmark dyes's dichloromethane excitation energies for the quantum methods: CAM-B3LYP/6-311G(d,p), BHandHLYP/6-311G(d,p), PBE0/6-311G(d,p) and the calculated LSF method with respect to the experiment.

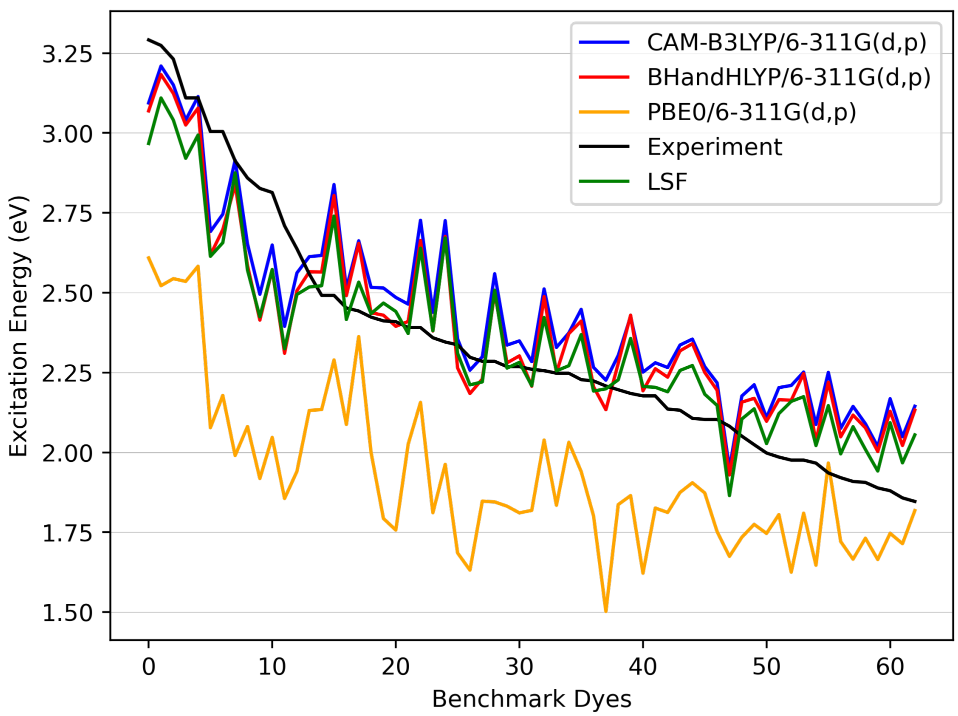


Figure S3: The benchmark dyes's tetrahydrofuran excitation energies for the quantum methods: CAM-B3LYP/6-311G(d,p), BHandHLYP/6-311G(d,p), PBE0/6-311G(d,p) and the calculated LSF method with respect to the experiment.

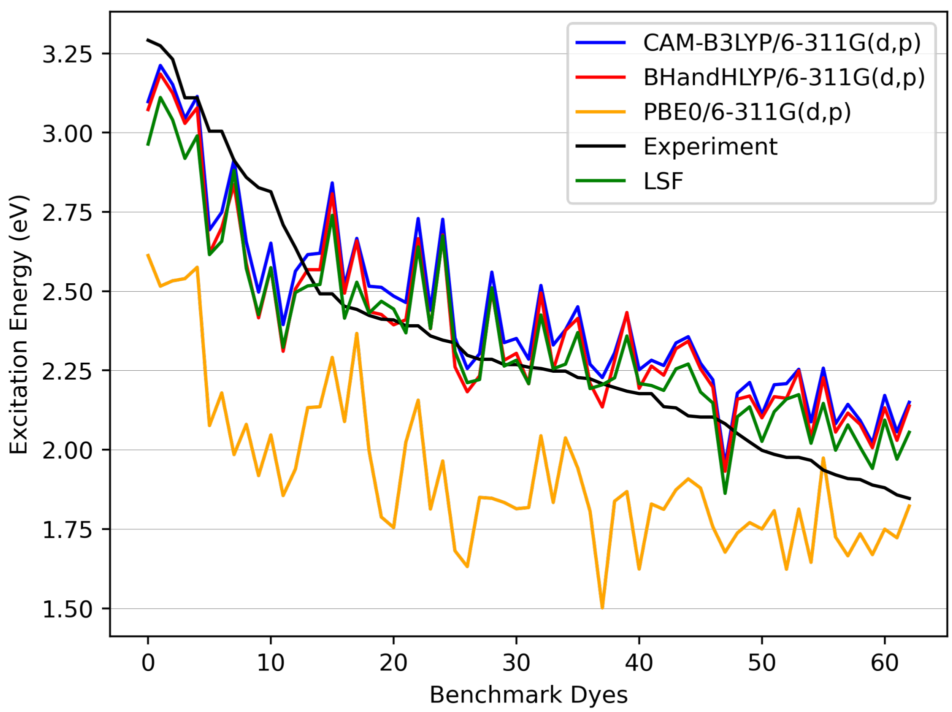


Figure S4: The benchmark dyes's N,N-dimethylformanide excitation energies for the quantum methods: CAM-B3LYP/6-311G(d,p), BHandHLYP/6-311G(d,p), PBE0/6-311G(d,p) and the calculated LSF method with respect to the experiment.

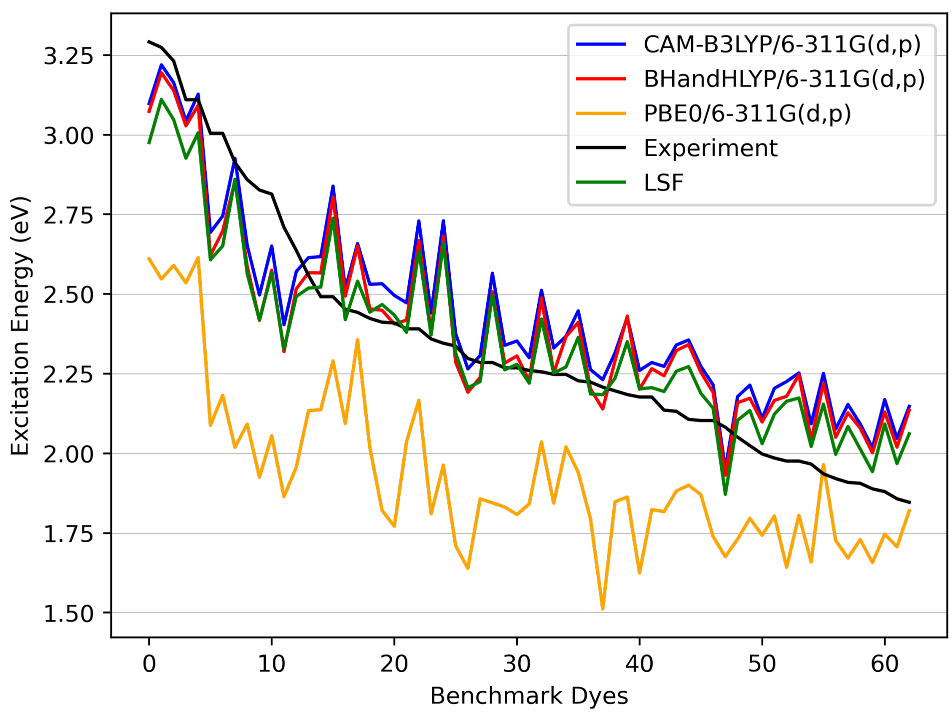


Figure S5: The π-bridge present in each theoretical dye with a LSF excitation energy less than FNE32. The light grey bars are 16b derivatives and the red bars are the 1b and 20b conjugated π-bridge. Lastly, the blue bars are other types of π-bridge involved with low energy absorbing dyes.

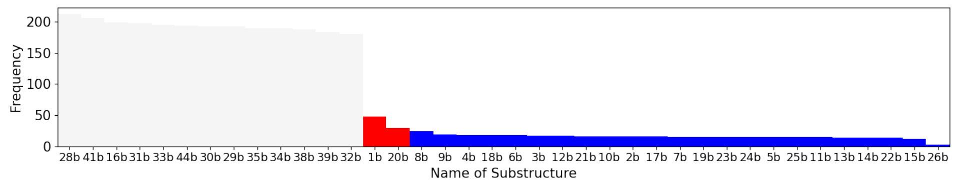


Table S6: The percentages and scoring for 800 to 1000

Name	HOMO Donor	LUMO Donor	HOMO Backbone	LUMO Backbone	HOMO Acceptor	LUMO Acceptor	HOMO Anchor	LUMO Anchor	HOMO Energy	LUMO energy	Wave	λ_{max} Score	LUMO Score	Charge Transfer Score	Total Score
22ed_16b_5ea	36	11	38	78	22	9	10	4	-5.06	-3.70	807	52	98	14	164
6ed_16b_5ea	32	12	41	78	27	9	13	4	-5.16	-3.60	803	51	84	13	147
9ed_29b_7ea	35	5	59	92	4	3	2	1	-4.87	-3.75	853	63	100	10	0
7ed_29b_9ea	14	5	71	87	15	8	4	2	-4.90	-3.74	856	64	100	8	0
7ed_29b_7ea	15	4	78	93	6	2	3	1	-4.85	-3.53	852	63	68	5	0
7ed_29b_6ea	16	4	77	92	7	3	3	2	-5.00	-3.78	847	62	98	6	0
7ed_29b_5ea	14	5	73	90	12	5	6	2	-4.95	-3.80	862	66	94	7	0
7ed_29b_2ea	16	4	77	91	7	4	3	2	-4.98	-3.77	847	62	100	6	0
7ed_29b_11ea	16	5	75	91	9	4	3	2	-5.00	-3.81	844	61	92	6	0
7ed_29b_10ea	15	5	75	91	9	4	1	0	-4.97	-3.76	845	61	100	6	0
7ed_28b_7ea	18	4	76	93	5	3	2	1	-4.97	-3.70	850	62	98	6	0
6ed_29b_9ea	18	5	72	91	9	4	4	2	-4.92	-3.68	846	62	96	7	0
6ed_29b_7ea	19	4	75	93	6	2	2	1	-4.78	-3.44	867	67	47	6	0
6ed_29b_6ea	19	5	74	92	6	3	3	2	-4.91	-3.68	865	66	96	7	0
6ed_29b_5ea	18	5	71	89	11	5	5	2	-4.88	-3.73	880	70	100	8	0
6ed_29b_2ea	19	5	74	91	7	4	3	2	-4.90	-3.69	866	66	97	7	0
6ed_29b_11ea	19	5	73	91	8	4	3	2	-4.90	-3.70	868	67	98	7	0
6ed_29b_10ea	18	5	73	91	8	4	1	0	-4.90	-3.64	844	61	90	6	0
6ed_28b_7ea	23	4	72	93	5	2	2	1	-4.85	-3.61	872	68	86	7	0
6ed_28b_5ea	20	5	69	90	10	5	5	3	-4.90	-3.85	900	75	80	8	0
6ed_28b_2ea	21	5	72	91	6	4	3	2	-4.95	-3.81	875	69	92	8	0
5ed_29b_7ea	33	3	62	94	5	3	2	1	-4.90	-3.66	826	57	94	10	0
5ed_28b_7ea	32	4	63	94	5	2	2	1	-4.99	-3.80	832	58	95	9	0
3ed_29b_9ea	12	4	77	92	10	4	5	2	-4.97	-3.85	860	65	81	6	0
3ed_29b_7ea	13	3	80	94	7	2	3	1	-4.88	-3.57	854	64	77	5	0
3ed_29b_6ea	13	4	80	93	7	3	3	2	-5.07	-3.85	836	59	82	5	0
3ed_29b_5ea	12	4	75	91	13	5	6	2	-4.96	-3.76	841	60	100	6	0
3ed_29b_10ea	13	4	78	92	9	4	1	0	-5.01	-3.83	850	62	86	5	0
3ed_28b_7ea	15	3	79	94	6	3	2	1	-5.07	-3.80	832	58	95	5	0
2ed_28b_7ea	19	3	76	94	5	3	2	1	-5.07	-3.83	828	57	88	6	0
22ed_29b_7ea	21	3	72	95	4	2	2	1	-4.79	-3.51	850	62	63	6	0
22ed_28b_7ea	25	3	69	94	4	2	1	1	-4.91	-3.62	820	55	87	8	0
22ed_26b_11ea	20	2	78	96	0	2	0	0	-5.04	-3.60	903	76	84	6	0
21ed_29b_9ea	9	3	75	88	16	9	4	3	-5.03	-3.83	823	56	86	7	0

21ed_29b_7ea	11	3	82	94	7	3	3	1	-5.05	-3.68	800	50	96	4	0
21ed_29b_6ea	9	3	83	94	7	3	3	1	-5.12	-3.81	805	51	92	4	0
21ed_29b_11ea	10	3	81	92	9	5	2	2	-5.08	-3.83	816	54	87	5	0
21ed_29b_10ea	9	3	81	92	10	4	1	0	-5.07	-3.81	815	54	92	5	0
21ed_28b_7ea	10	3	84	95	6	3	2	1	-4.99	-3.68	835	59	96	4	0
20ed_29b_9ea	16	3	68	87	13	9	3	2	-4.92	-3.82	854	64	91	9	0
20ed_29b_7ea	17	3	75	94	6	3	2	1	-4.86	-3.58	845	61	79	6	0
20ed_29b_6ea	18	3	73	93	6	3	3	1	-5.03	-3.85	832	58	81	6	0
20ed_29b_5ea	16	3	71	91	12	5	6	3	-4.94	-3.77	837	59	100	7	0
20ed_29b_10ea	18	3	71	92	8	4	1	0	-4.98	-3.83	842	61	87	7	0
20ed_28b_7ea	18	3	75	94	6	2	2	1	-4.99	-3.74	837	59	100	6	0
1ed_29b_7ea	22	4	72	94	6	3	2	1	-5.00	-3.78	829	57	99	7	0
19ed_29b_7ea	9	3	84	95	7	3	3	1	-5.09	-3.81	818	55	94	4	0
17ed_29b_7ea	13	4	80	94	7	2	3	1	-5.08	-3.82	813	53	89	5	0
16ed_29b_9ea	17	5	70	87	13	8	3	2	-4.93	-3.78	860	65	98	9	0
16ed_29b_7ea	19	4	75	93	6	3	2	1	-4.97	-3.66	833	58	93	6	0
16ed_29b_11ea	18	5	74	91	8	4	2	1	-5.04	-3.80	821	55	95	7	0
16ed_29b_10ea	18	5	73	91	8	4	1	0	-5.00	-3.81	847	62	91	7	0
16ed_28b_7ea	24	3	71	94	5	3	2	1	-5.05	-3.83	831	58	87	8	0
13ed_29b_7ea	24	5	70	93	6	2	2	1	-5.02	-3.83	828	57	88	7	0
11ed_29b_7ea	35	5	60	92	5	3	2	1	-4.94	-3.81	843	61	92	10	0
10ed_29b_9ea	22	4	68	91	9	5	4	2	-4.95	-3.81	846	61	91	8	0
10ed_29b_7ea	20	3	73	94	6	3	2	1	-4.86	-3.58	846	61	79	7	0
10ed_29b_10ea	21	4	69	92	8	4	1	0	-4.97	-3.82	845	61	88	8	0
10ed_28b_7ea	23	3	70	94	5	3	2	1	-4.97	-3.74	839	60	100	7	0

Table S7: The percentages and scoring for 600 to 800

Name	HOMO Donor	LUMO Donor	HOMO Backbone	LUMO Backbone	HOMO Acceptor	LUMO Acceptor	HOMO Anchor	LUMO Anchor	HOMO Energy	LUMO energy	Wave	λ_{max} Score	LUMO Score	Charge Transfer Score	Total Score
10ed_16b_9ea	32	11	34	74	32	14	9	4	-5.14	-3.74	755	39	100	16	154
23ed_9b_4ea	64	13	22	38	10	48	3	13	-5.18	-3.72	641	10	99	43	152
23ed_20b_4ea	67	16	19	47	11	35	3	9	-5.08	-3.82	706	26	90	36	152
6ed_8b_12ea	27	8	36	41	36	50	12	12	-5.36	-3.75	665	16	100	34	151
22ed_16b_2ea	44	12	40	79	12	8	6	4	-5.24	-3.71	746	36	99	15	151
10ed_20b_12ea	33	11	28	47	37	39	12	10	-5.28	-3.74	681	20	100	30	150
5ed_16b_9ea	46	11	28	72	26	17	7	4	-5.14	-3.82	753	38	89	20	148
9ed_9b_12ea	60	15	20	35	17	50	5	12	-5.30	-3.80	638	9	95	42	147
20ed_16b_5ea	30	9	39	79	27	9	13	5	-5.21	-3.82	780	45	89	13	147
2ed_9b_12ea	20	9	40	37	40	54	12	13	-5.47	-3.72	642	11	99	35	145
6ed_1b_12ea	27	12	30	53	42	34	13	8	-5.36	-3.70	683	21	98	25	144
20ed_16b_9ea	32	9	39	80	24	9	11	4	-5.29	-3.78	725	31	99	13	143
9ed_20b_1ea	68	18	20	48	9	33	3	11	-5.20	-3.68	643	11	96	36	142
23ed_20b_1ea	72	15	18	48	6	35	2	11	-5.09	-3.65	650	13	92	38	142
23ed_1b_3ea	77	21	15	63	4	16	2	8	-5.19	-3.79	664	16	97	28	141
5ed_16b_2ea	60	12	30	78	10	9	5	4	-5.26	-3.69	693	23	97	20	140
11ed_20b_1ea	73	18	17	48	7	32	2	11	-5.30	-3.79	624	6	97	37	139
5ed_9b_12ea	43	8	30	35	26	57	8	14	-5.37	-3.64	621	5	91	42	138
11ed_1b_5ea	67	18	19	65	12	15	6	7	-5.25	-3.68	658	15	97	25	137
5ed_20b_12ea	49	12	22	47	27	40	9	10	-5.28	-3.84	677	19	83	34	136
11ed_26b_8ea	91	1	5	75	0	23	0	14	-5.36	-3.65	626	7	93	37	136
7ed_1b_12ea	18	12	31	61	51	27	16	6	-5.39	-3.76	667	17	100	19	135

20ed_20b_4ea	37	9	34	47	24	41	9	12	-5.41	-3.67	627	7	95	33	135
20ed_20b_12ea	32	8	30	42	33	47	10	12	-5.40	-3.66	629	7	94	34	135
23ed_1b_1ea	72	17	18	54	6	28	2	8	-5.16	-3.85	680	20	80	34	134
11ed_1b_9ea	63	17	19	56	16	26	4	7	-5.22	-3.65	646	12	92	30	134
11ed_1b_3ea	77	20	15	66	5	14	2	6	-5.35	-3.76	623	6	100	28	133
1ed_20b_4ea	53	10	27	50	19	39	2	5	-5.46	-3.70	601	0	98	34	132
20ed_16b_2ea	38	10	42	81	15	8	7	4	-5.41	-3.83	719	30	87	14	131
16ed_20b_4ea	42	10	34	47	23	41	8	12	-5.52	-3.66	617	4	93	34	131
6ed_1b_4ea	36	12	36	56	27	31	10	9	-5.45	-3.64	654	14	90	27	130
5ed_20b_4ea	61	11	23	52	15	36	2	5	-5.30	-3.64	624	6	91	34	130
13ed_1b_5ea	62	16	23	66	15	16	7	9	-5.35	-3.67	642	11	94	25	130
10ed_20b_4ea	43	10	32	50	22	38	8	11	-5.39	-3.64	629	7	90	32	130
11ed_1b_11ea	73	20	17	68	8	12	3	5	-5.34	-3.70	621	5	98	25	129
23ed_20b_8ea	74	24	15	56	7	17	7	11	-5.24	-3.84	659	15	84	29	128
16ed_9b_12ea	30	9	36	35	33	56	10	13	-5.48	-3.61	616	4	86	38	128
2ed_20b_4ea	32	10	39	51	28	39	10	11	-5.57	-3.66	617	4	93	30	127
2ed_20b_12ea	26	9	34	43	40	46	12	11	-5.53	-3.64	617	4	91	32	127
22ed_20b_4ea	44	10	33	45	19	43	6	12	-5.25	-3.58	652	13	79	35	127
1ed_20b_12ea	50	10	25	43	25	46	7	12	-5.49	-3.83	613	3	86	38	127
9ed_26b_8ea	85	1	11	76	0	23	0	14	-5.31	-3.61	624	6	85	36	126
22ed_1b_8ea	53	15	29	67	13	17	13	11	-5.57	-3.74	606	1	100	24	125
11ed_20b_3ea	75	20	16	60	5	18	3	7	-5.35	-3.68	602	1	96	29	125
10ed_1b_1ea	52	10	32	56	13	33	4	11	-5.49	-3.65	604	1	93	32	125
16ed_1b_1ea	51	11	34	57	15	32	4	11	-5.63	-3.65	602	1	92	31	124
3ed_1b_4ea	21	11	41	64	38	24	14	7	-5.62	-3.80	629	7	95	19	121
16ed_20b_12ea	36	10	30	43	33	46	10	11	-5.50	-3.60	611	3	83	34	120
22ed_1b_1ea	51	10	33	53	11	36	3	11	-5.35	-3.58	625	6	79	33	119
7ed_1b_4ea	25	13	39	65	35	21	12	6	-5.50	-3.62	636	9	88	18	115
6ed_26b_8ea	43	1	53	75	2	23	2	14	-5.18	-3.61	619	5	85	25	115
21ed_16b_5ea	14	11	51	77	34	11	17	5	-5.52	-3.63	662	16	89	10	114
23ed_1b_2ea	77	20	15	66	4	14	2	7	-5.10	-3.55	652	13	73	27	113
9ed_1b_9ea	59	18	21	55	18	27	5	7	-5.12	-3.53	659	15	67	30	111
14ed_8b_9ea	92	4	1	26	2	69	0	4	-5.42	-3.34	707	27	26	58	111
9ed_1b_11ea	69	21	20	67	9	12	3	5	-5.23	-3.57	636	9	76	24	109
3ed_20b_4ea	20	10	42	59	37	29	14	8	-5.49	-3.59	620	5	81	21	107
1ed_26b_8ea	3	1	91	75	5	24	4	14	-5.29	-3.60	626	7	84	16	107
3ed_9b_12ea	16	9	40	38	43	53	13	12	-5.44	-3.53	620	5	68	33	106
21ed_16b_9ea	12	8	43	66	44	25	13	5	-5.45	-3.58	639	10	80	16	106
3ed_20b_12ea	17	10	34	48	49	40	15	10	-5.44	-3.56	619	5	74	26	105
21ed_16b_2ea	20	10	60	80	19	9	9	5	-5.82	-3.65	606	1	92	11	104
11ed_1b_2ea	76	19	17	68	5	12	2	5	-5.28	-3.55	618	4	72	26	102
3ed_26b_8ea	9	1	87	74	4	24	3	14	-5.29	-3.58	612	3	79	17	100
23ed_20b_3ea	75	19	16	60	4	19	2	10	-5.13	-3.51	629	7	63	30	100
23ed_1b_9ea	64	18	20	57	13	25	3	6	-5.02	-3.47	667	17	53	30	100
6ed_9b_12ea	28	10	36	36	34	53	11	13	-5.33	-3.47	638	10	52	37	99
7ed_26b_8ea	17	1	79	73	3	24	2	14	-5.21	-3.55	618	5	73	20	97
6ed_20b_12ea	31	11	32	43	36	45	11	11	-5.34	-3.46	642	11	51	32	94
9ed_1b_6ea	71	19	20	70	6	10	3	5	-5.23	-3.50	631	8	61	24	93
2ed_26b_8ea	17	1	79	76	3	22	3	22	-5.30	-3.54	603	1	71	20	92
6ed_20b_4ea	36	12	36	53	27	34	10	10	-5.35	-3.46	649	12	51	28	91
10ed_26b_8ea	5	1	90	73	4	26	3	15	-5.24	-3.51	632	8	64	17	89
6ed_9b_4ea	37	8	41	31	21	61	7	18	-5.38	-3.41	601	0	41	44	85
23ed_1b_6ea	74	19	18	69	5	11	2	5	-5.12	-3.45	640	10	49	25	84

7ed_9b_12ea	19	9	38	38	43	52	13	12	-5.32	-3.42	635	9	41	33	83
7ed_20b_12ea	20	11	33	48	47	38	15	9	-5.32	-3.44	633	8	47	26	82
22ed_13b_9ea	40	3	32	15	24	82	0	7	-5.28	-3.13	702	26	5	52	82
22ed_11b_9ea	38	4	29	12	29	83	0	8	-5.04	-2.67	700	25	0	53	78
20ed_17b_9ea	29	2	26	5	41	93	0	9	-5.27	-2.88	691	23	0	56	78
11ed_20b_9ea	68	20	20	62	10	16	5	7	-5.16	-3.44	621	5	47	26	78
6ed_1b_1ea	44	12	38	56	17	32	5	11	-5.47	-3.43	615	4	43	29	76
20ed_7b_9ea	26	2	23	8	48	89	0	11	-5.37	-2.91	688	22	0	53	76
16ed_17b_9ea	26	3	27	8	47	89	0	8	-5.30	-2.86	693	23	0	52	76
7ed_20b_4ea	25	11	40	58	35	29	13	8	-5.37	-3.44	626	7	46	22	75
6ed_8b_9ea	30	6	40	33	29	60	8	18	-5.17	-3.11	716	29	4	42	75
16ed_6b_9ea	23	1	43	14	34	84	0	7	-5.24	-3.00	694	23	1	49	74
19ed_9b_9ea	8	5	36	24	56	71	0	5	-5.36	-3.18	711	28	7	38	73
19ed_12b_9ea	8	3	27	6	65	91	0	9	-5.43	-2.86	694	24	0	49	73
9ed_20b_3ea	71	21	19	59	7	18	3	7	-5.18	-3.40	623	6	38	28	72
9ed_1b_2ea	71	20	20	67	6	12	3	5	-5.17	-3.41	632	8	39	25	72
22ed_1b_3ea	55	13	31	69	8	18	4	9	-5.42	-3.44	605	1	46	24	72
22ed_14b_9ea	48	4	22	19	25	76	0	6	-5.19	-2.84	682	21	0	51	72
21ed_10b_9ea	8	2	48	13	43	86	0	7	-5.12	-2.86	702	26	0	46	72
20ed_3b_9ea	21	1	53	21	24	79	0	6	-5.32	-3.15	686	21	6	45	72
17ed_6b_9ea	11	2	43	15	46	83	0	6	-5.34	-3.08	696	24	3	45	72
21ed_13b_9ea	9	2	33	12	57	86	0	7	-5.41	-2.97	691	23	1	47	70
11ed_20b_5ea	64	20	21	60	13	17	6	9	-5.19	-3.39	629	7	36	26	70
9ed_20b_5ea	60	20	23	59	14	17	7	9	-5.09	-3.36	654	13	30	25	69
7ed_1b_1ea	32	12	44	65	23	23	8	8	-5.52	-3.44	608	2	46	21	69
21ed_2b_9ea	8	1	43	15	49	84	0	7	-5.38	-3.01	690	23	1	45	69
13ed_20b_9ea	53	15	25	49	22	34	6	10	-5.27	-3.40	600	0	37	32	69
2ed_26b_9ea	8	1	80	61	11	37	3	12	-5.10	-3.38	624	6	33	23	62
13ed_20b_5ea	62	17	25	63	12	17	6	9	-5.31	-3.39	608	2	35	26	62
23ed_20b_9ea	63	17	21	54	13	27	3	8	-4.95	-3.29	645	11	18	31	60
9ed_20b_9ea	53	19	25	48	21	31	6	9	-5.05	-3.30	632	8	20	31	58
3ed_21b_9ea	23	5	28	40	48	54	16	17	-5.46	-2.91	685	21	0	36	58
9ed_20b_11ea	67	22	21	61	9	15	3	6	-5.17	-3.35	618	4	28	25	57
23ed_20b_5ea	65	18	21	62	10	16	5	8	-4.98	-3.27	658	14	16	26	56
23ed_20b_2ea	74	19	18	64	5	15	2	8	-5.04	-3.29	628	7	18	27	53
1ed_26b_9ea	2	1	85	59	13	40	3	13	-5.07	-3.31	622	5	21	23	49
5ed_1b_5ea	62	11	24	71	14	16	7	8	-5.28	-3.30	603	1	20	25	46
9ed_20b_6ea	69	20	22	67	7	11	3	6	-5.16	-3.28	615	4	17	24	44
2ed_26b_11ea	11	2	83	82	5	16	2	7	-5.20	-3.36	611	3	29	12	44
16ed_1b_5ea	49	11	33	72	19	15	9	8	-5.48	-3.30	602	1	20	21	42
2ed_1b_5ea	36	10	40	72	24	16	12	9	-5.53	-3.31	606	2	21	19	41
3ed_26b_11ea	7	2	87	82	6	16	2	7	-5.17	-3.33	613	3	24	11	38
22ed_1b_9ea	42	10	32	56	22	32	5	8	-5.14	-3.15	617	4	6	28	38
10ed_1b_5ea	45	11	33	70	20	17	10	9	-5.28	-3.22	620	5	11	21	37
9ed_26b_11ea	30	1	64	81	4	17	1	7	-5.18	-3.28	609	2	17	17	36
20ed_1b_5ea	37	9	35	72	22	16	11	8	-5.35	-3.24	609	2	13	19	34
9ed_20b_2ea	70	21	21	62	7	15	3	6	-5.11	-3.14	606	1	5	26	33
6ed_26b_9ea	34	2	61	79	4	18	2	9	-5.07	-3.24	608	2	12	19	33
22ed_1b_5ea	45	12	34	69	17	16	8	8	-5.18	-3.14	631	8	5	21	33
6ed_1b_5ea	39	12	37	73	23	13	11	7	-5.34	-3.15	632	8	6	17	31
3ed_26b_9ea	6	1	86	79	7	18	3	9	-5.14	-3.27	613	3	16	12	31
10ed_26b_9ea	3	1	85	57	12	42	3	12	-5.06	-3.12	608	2	4	24	31
1ed_26b_11ea	3	1	90	81	6	17	2	7	-5.17	-3.27	607	2	16	11	29

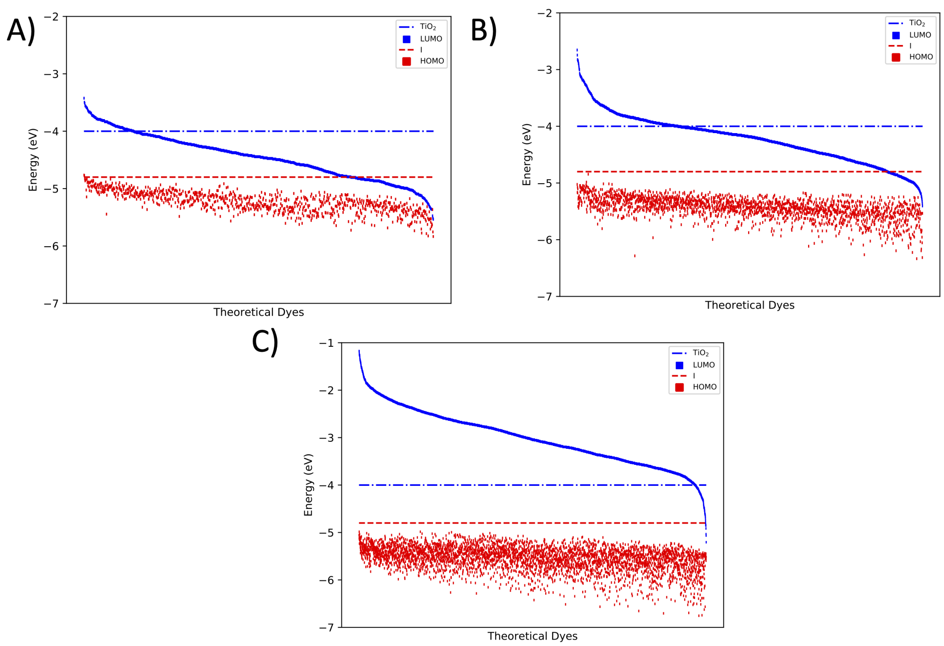
7ed_26b_9ea	13	2	81	78	5	18	2	9	-5.06	-3.20	617	4	9	14	28
5ed_26b_9ea	4	1	88	78	7	20	3	10	-5.10	-3.17	609	2	7	13	22
5ed_26b_11ea	2	1	90	82	7	17	2	8	-5.13	-3.21	610	3	10	10	22
22ed_20b_5ea	44	12	35	64	17	19	8	9	-5.09	-2.84	600	0	0	22	22
10ed_26b_11ea	4	1	90	81	6	18	2	8	-5.10	-3.20	609	2	9	12	22
6ed_20b_5ea	39	11	37	71	23	14	11	8	-5.26	-2.94	610	3	1	18	21
3ed_1b_5ea	22	11	44	78	34	9	17	5	-5.41	-3.17	613	3	7	11	21
7ed_1b_5ea	26	11	42	78	31	9	16	5	-5.29	-3.02	623	6	1	12	19
7ed_20b_5ea	25	11	43	74	31	11	15	6	-5.18	-2.76	601	0	0	13	13
9ed_31b_7ea	67	3	29	95	1	2	0	0	-5.12	-3.75	703	26	100	18	0
9ed_20b_10ea	66	22	22	61	10	15	1	2	-5.12	-3.21	610	2	10	25	0
9ed_1b_7ea	68	19	22	73	7	8	3	3	-5.09	-3.11	619	5	4	22	0
7ed_35b_7ea	20	1	79	98	1	1	0	0	-5.24	-3.83	702	26	86	5	0
7ed_34b_7ea	19	2	79	97	2	1	1	0	-5.22	-3.74	708	27	100	5	0
7ed_33b_6ea	23	2	75	97	2	1	1	1	-5.25	-3.82	731	33	91	6	0
7ed_33b_5ea	21	2	75	96	4	3	2	1	-5.21	-3.80	737	34	94	7	0
7ed_33b_2ea	23	2	74	96	2	2	1	1	-5.22	-3.79	731	33	98	7	0
7ed_33b_10ea	22	2	75	96	3	2	0	0	-5.24	-3.83	735	34	87	6	0
7ed_32b_9ea	22	4	65	89	12	7	3	2	-5.34	-3.80	701	25	95	10	0
7ed_32b_7ea	25	3	71	96	3	2	1	0	-5.31	-3.57	688	22	76	7	0
7ed_32b_6ea	27	3	69	95	3	3	1	1	-5.42	-3.77	687	22	99	8	0
7ed_32b_5ea	23	3	68	92	8	5	4	3	-5.36	-3.81	702	25	94	9	0
7ed_32b_2ea	27	3	69	92	3	4	1	2	-5.37	-3.73	689	22	100	9	0
7ed_32b_10ea	24	3	69	93	6	3	0	0	-5.39	-3.83	698	24	88	8	0
7ed_31b_9ea	23	3	70	93	6	3	3	1	-5.24	-3.81	750	38	93	8	0
7ed_31b_7ea	23	3	73	96	3	1	1	0	-5.15	-3.53	741	35	67	7	0
7ed_31b_6ea	24	3	72	94	3	2	1	1	-5.26	-3.74	739	35	100	7	0
7ed_31b_5ea	22	3	70	92	8	4	4	2	-5.20	-3.75	754	38	100	8	0
7ed_31b_3ea	25	3	71	92	4	4	2	2	-5.27	-3.82	744	36	90	9	0
7ed_31b_2ea	23	3	73	93	4	3	2	1	-5.20	-3.68	742	36	96	8	0
7ed_31b_11ea	23	3	71	94	6	3	2	1	-5.27	-3.84	747	37	84	8	0
7ed_31b_10ea	23	3	71	94	6	3	0	0	-5.24	-3.79	750	37	97	7	0
7ed_26b_10ea	13	2	81	80	5	17	0	2	-5.07	-3.20	615	4	9	12	0
7ed_16b_9ea	22	10	44	71	32	19	15	2	-5.28	-3.58	722	30	80	15	0
7ed_16b_7ea	34	7	50	88	15	5	6	2	-5.34	-3.43	714	28	44	11	0
7ed_16b_6ea	27	12	52	84	20	4	9	2	-5.37	-3.62	738	34	88	9	0
7ed_16b_3ea	26	13	52	83	21	4	10	2	-5.50	-3.68	696	24	96	9	0
7ed_16b_2ea	30	11	52	84	18	5	8	2	-5.43	-3.57	710	28	77	10	0
7ed_16b_11ea	24	11	48	77	27	12	9	1	-5.37	-3.68	715	29	96	12	0
7ed_16b_10ea	28	7	47	66	24	26	2	0	-5.40	-3.69	714	29	97	20	0
6ed_35b_7ea	36	1	62	98	1	1	0	0	-5.19	-3.82	695	24	90	9	0
6ed_34b_7ea	31	2	67	97	2	1	0	0	-5.16	-3.74	706	27	100	8	0
6ed_33b_9ea	36	2	60	96	3	3	1	1	-5.13	-3.80	758	40	94	11	0
6ed_33b_6ea	40	2	58	97	1	1	0	1	-5.20	-3.83	722	31	87	11	0
6ed_33b_3ea	40	2	58	95	1	3	1	1	-5.18	-3.83	724	31	88	12	0
6ed_33b_10ea	38	2	59	96	2	2	0	0	-5.17	-3.82	729	32	90	10	0
6ed_32b_9ea	35	4	56	87	8	9	2	3	-5.22	-3.78	717	29	98	14	0
6ed_32b_7ea	41	3	56	95	2	2	1	1	-5.21	-3.55	689	22	73	11	0
6ed_32b_6ea	42	3	55	94	2	2	1	1	-5.31	-3.75	689	22	100	12	0
6ed_32b_5ea	34	4	59	89	6	7	3	3	-5.27	-3.80	706	27	95	13	0
6ed_32b_3ea	41	4	55	91	3	5	1	2	-5.32	-3.83	696	24	87	14	0
6ed_32b_2ea	41	4	56	91	3	5	1	2	-5.28	-3.66	670	17	93	13	0
6ed_32b_11ea	40	4	55	92	4	4	1	2	-5.34	-3.84	682	20	84	13	0

6ed_32b_10ea	40	4	55	93	4	4	0	0	-5.30	-3.81	700	25	93	12	0
6ed_31b_9ea	32	4	59	90	9	6	2	2	-5.12	-3.74	756	39	100	11	0
6ed_31b_7ea	36	3	60	95	3	1	1	0	-5.09	-3.55	741	35	72	10	0
6ed_31b_6ea	38	3	59	94	3	2	1	1	-5.18	-3.73	741	35	100	11	0
6ed_31b_5ea	33	4	60	92	6	4	3	2	-5.13	-3.74	756	39	100	11	0
6ed_31b_3ea	36	4	60	92	3	4	1	2	-5.18	-3.78	745	36	98	12	0
6ed_31b_2ea	35	4	61	93	3	3	1	1	-5.13	-3.65	743	36	92	11	0
6ed_31b_10ea	35	4	60	93	5	3	0	0	-5.16	-3.77	752	38	100	10	0
6ed_26b_10ea	35	2	60	81	4	16	0	2	-5.12	-3.22	605	1	10	17	0
6ed_18b_9ea	44	8	20	51	35	41	0	2	-5.44	-3.48	684	21	55	32	0
6ed_16b_9ea	32	7	42	50	25	43	12	2	-5.23	-3.48	737	34	57	30	0
6ed_16b_7ea	41	11	44	84	14	5	5	2	-5.16	-3.27	748	37	16	13	0
6ed_16b_6ea	39	12	45	81	15	7	7	2	-5.34	-3.59	748	37	81	14	0
6ed_16b_3ea	35	15	47	79	18	6	8	2	-5.39	-3.54	722	31	71	12	0
6ed_16b_2ea	36	14	47	80	17	5	8	2	-5.26	-3.36	734	34	30	12	0
6ed_16b_11ea	34	7	43	50	22	42	7	1	-5.31	-3.58	733	33	80	30	0
6ed_16b_10ea	34	7	43	51	23	42	2	0	-5.24	-3.51	743	36	62	29	0
5ed_33b_7ea	72	1	27	98	1	1	0	0	-5.24	-3.75	692	23	100	18	0
5ed_32b_2ea	78	3	20	92	1	5	0	2	-5.37	-3.84	616	4	84	22	0
5ed_32b_10ea	75	3	22	93	1	4	0	1	-5.37	-3.81	612	3	94	21	0
5ed_31b_7ea	70	2	28	97	1	1	0	0	-5.24	-3.70	687	22	98	18	0
5ed_26b_10ea	3	1	90	80	7	19	0	2	-5.09	-3.14	607	2	5	11	0
5ed_16b_7ea	59	10	30	84	10	6	4	2	-5.12	-3.51	725	31	63	18	0
5ed_16b_10ea	56	11	29	80	14	8	1	1	-5.23	-3.80	726	31	94	18	0
3ed_34b_7ea	15	2	83	97	2	1	1	0	-5.29	-3.81	702	26	92	4	0
3ed_32b_7ea	22	3	74	95	4	2	1	0	-5.39	-3.64	681	20	91	6	0
3ed_31b_7ea	19	3	77	96	4	1	1	0	-5.23	-3.62	732	33	87	6	0
3ed_31b_6ea	20	3	76	95	3	2	1	1	-5.35	-3.83	730	32	87	6	0
3ed_26b_10ea	4	2	87	82	8	15	1	2	-5.18	-3.23	606	2	12	9	0
3ed_16b_9ea	19	9	45	75	35	16	16	2	-5.40	-3.73	706	26	100	13	0
3ed_16b_7ea	24	10	55	87	21	3	8	1	-5.26	-3.40	741	35	37	8	0
3ed_16b_6ea	23	10	55	87	22	3	10	2	-5.50	-3.77	723	31	99	8	0
3ed_16b_3ea	22	11	55	84	22	4	11	2	-5.62	-3.83	688	22	87	8	0
3ed_16b_2ea	22	11	56	86	22	4	10	2	-5.48	-3.61	699	25	86	8	0
3ed_16b_11ea	21	10	50	81	29	9	10	1	-5.48	-3.82	706	26	91	10	0
3ed_16b_10ea	21	10	50	80	29	10	2	0	-5.40	-3.71	710	28	98	10	0
2ed_33b_7ea	26	1	72	98	2	1	0	0	-5.27	-3.77	712	28	100	7	0
2ed_32b_7ea	32	3	65	96	3	2	1	0	-5.39	-3.70	675	19	98	9	0
2ed_26b_10ea	10	2	83	81	6	16	0	2	-5.15	-3.27	609	2	15	11	0
2ed_16b_9ea	28	6	45	53	26	40	13	2	-5.46	-3.77	712	28	100	28	0
2ed_16b_7ea	36	8	49	85	15	6	6	2	-5.45	-3.54	702	25	71	13	0
2ed_16b_6ea	34	10	50	83	16	7	7	3	-5.58	-3.84	717	29	83	13	0
2ed_16b_3ea	32	13	50	80	18	7	8	3	-5.59	-3.80	709	27	94	12	0
2ed_16b_2ea	33	12	50	81	17	6	8	2	-5.49	-3.63	712	28	89	12	0
2ed_16b_11ea	30	6	47	53	23	40	7	1	-5.53	-3.85	711	28	81	28	0
2ed_16b_10ea	30	6	47	53	23	40	2	0	-5.47	-3.76	713	28	100	28	0
23ed_8b_8ea	78	20	12	51	5	29	5	17	-5.28	-3.95	616	4	0	38	0
23ed_8b_4ea	73	10	16	36	7	53	2	14	-5.17	-3.99	636	9	0	48	0
23ed_4b_4ea	82	12	9	50	4	38	1	11	-5.25	-3.98	612	3	0	42	0
23ed_22b_8ea	84	20	8	63	2	15	2	9	-5.26	-3.87	601	0	0	31	0
23ed_20b_7ea	70	19	21	70	5	9	2	3	-4.91	-2.83	607	2	0	23	0
23ed_20b_10ea	70	19	20	64	7	15	0	2	-5.00	-3.21	626	6	10	25	0
23ed_1b_7ea	71	19	20	72	5	9	2	3	-4.98	-3.05	625	6	2	23	0

23ed_1b_10ea	72	19	18	67	7	14	0	1	-5.06	-3.42	645	11	42	25	0
23ed_19b_9ea	79	12	10	32	7	54	0	2	-5.08	-3.27	668	17	16	47	0
23ed_18b_9ea	80	11	9	63	7	25	0	0	-5.13	-3.79	675	19	97	33	0
23ed_16b_7ea	63	15	27	79	8	6	3	2	-4.91	-3.64	796	49	91	19	0
23ed_16b_11ea	60	18	26	73	11	9	2	3	-5.08	-3.99	796	49	0	20	0
22ed_8b_9ea	35	5	36	35	26	59	0	3	-5.14	-3.20	713	28	9	39	0
22ed_33b_7ea	37	1	58	98	1	1	0	0	-5.17	-3.71	707	27	99	10	0
22ed_31b_7ea	39	2	55	97	2	1	1	0	-5.14	-3.58	707	27	79	11	0
22ed_26b_10ea	8	1	83	91	7	6	0	0	-4.86	-3.37	757	39	31	5	0
22ed_16b_9ea	33	11	36	73	28	15	6	3	-5.03	-3.66	778	44	94	16	0
22ed_16b_7ea	42	10	41	84	12	6	5	2	-5.00	-3.30	760	40	20	14	0
22ed_16b_6ea	43	11	40	81	12	7	5	3	-5.19	-3.68	758	40	96	15	0
22ed_16b_11ea	40	12	39	79	17	8	3	3	-5.17	-3.70	751	38	98	15	0
22ed_16b_10ea	40	11	39	80	17	8	1	1	-5.13	-3.64	753	38	91	14	0
21ed_33b_7ea	4	1	93	98	3	1	1	0	-5.39	-3.78	711	28	98	1	0
21ed_32b_7ea	8	1	87	97	5	2	2	1	-5.50	-3.59	659	15	81	3	0
21ed_32b_6ea	9	1	86	96	5	3	2	1	-5.64	-3.82	655	14	89	4	0
21ed_32b_10ea	7	2	83	94	9	4	1	0	-5.61	-3.83	644	11	88	4	0
21ed_31b_7ea	8	1	87	97	5	2	2	0	-5.35	-3.58	704	26	80	3	0
21ed_31b_6ea	8	1	87	96	5	2	2	1	-5.49	-3.81	699	25	93	4	0
21ed_31b_5ea	7	2	81	94	12	4	6	2	-5.40	-3.84	714	29	84	4	0
21ed_16b_6ea	19	11	61	81	20	8	9	3	-5.74	-3.59	615	4	82	9	0
21ed_16b_11ea	17	10	56	74	26	17	6	3	-5.67	-3.63	615	4	89	13	0
21ed_16b_10ea	16	9	55	73	28	18	2	1	-5.62	-3.56	618	4	74	13	0
20ed_34b_7ea	25	1	70	98	2	1	1	0	-5.32	-3.84	687	22	82	7	0
20ed_33b_7ea	26	1	69	98	2	1	1	0	-5.29	-3.75	711	28	100	7	0
20ed_32b_7ea	35	2	58	96	3	2	1	1	-5.41	-3.65	658	14	93	10	0
20ed_31b_7ea	29	2	63	97	3	2	1	0	-5.27	-3.64	707	27	91	8	0
20ed_16b_7ea	37	8	44	86	14	6	6	2	-5.15	-3.42	732	33	42	13	0
20ed_16b_6ea	38	9	43	83	15	7	7	3	-5.36	-3.80	731	33	95	14	0
20ed_16b_11ea	35	10	41	81	20	9	4	3	-5.32	-3.81	722	30	92	14	0
20ed_16b_10ea	34	9	40	82	21	8	1	1	-5.28	-3.75	727	32	100	13	0
1ed_33b_7ea	38	1	60	98	2	1	1	0	-5.37	-3.85	708	27	81	10	0
1ed_32b_7ea	57	2	41	96	2	2	1	1	-5.51	-3.76	629	7	100	15	0
1ed_31b_7ea	46	2	51	96	3	2	1	0	-5.37	-3.78	697	24	98	12	0
1ed_26b_10ea	3	1	89	80	7	18	0	2	-5.12	-3.18	607	2	8	10	0
1ed_18b_9ea	82	6	9	61	8	33	0	2	-5.62	-3.83	674	19	88	37	0
1ed_16b_7ea	53	9	35	85	11	6	5	2	-5.29	-3.67	710	27	95	17	0
19ed_32b_7ea	9	2	86	96	5	2	2	1	-5.64	-3.82	657	14	90	3	0
19ed_31b_7ea	8	2	87	97	5	2	2	0	-5.48	-3.81	701	25	93	3	0
19ed_16b_7ea	25	7	56	86	19	6	8	3	-5.58	-3.76	680	20	100	10	0
17ed_32b_7ea	22	2	74	96	4	2	1	1	-5.60	-3.83	656	14	88	7	0
17ed_31b_7ea	17	2	79	96	5	2	1	0	-5.45	-3.82	702	25	91	5	0
17ed_16b_7ea	42	9	44	85	14	7	6	3	-5.48	-3.78	687	22	98	14	0
16ed_34b_7ea	31	2	67	97	2	1	1	0	-5.26	-3.84	699	25	84	8	0
16ed_33b_7ea	36	1	63	98	1	1	0	0	-5.23	-3.77	718	30	99	9	0
16ed_32b_7ea	41	3	56	95	2	2	1	0	-5.34	-3.68	676	19	96	11	0
16ed_31b_7ea	36	3	61	96	3	1	1	0	-5.21	-3.66	726	32	94	10	0
16ed_18b_9ea	48	7	18	54	34	38	0	1	-5.57	-3.71	680	20	99	31	0
16ed_16b_9ea	31	7	37	50	31	44	9	2	-5.28	-3.76	744	36	100	30	0
16ed_16b_7ea	47	9	41	85	12	6	5	2	-5.35	-3.51	713	28	64	15	0
16ed_16b_6ea	43	11	44	82	13	7	6	3	-5.50	-3.79	723	31	97	15	0
16ed_16b_2ea	39	13	45	80	16	6	8	3	-5.49	-3.70	719	30	98	14	0

16ed_16b_11ea	37	7	43	52	20	41	4	1	-5.42	-3.74	723	31	100	30	0
16ed_16b_10ea	36	7	42	53	21	41	1	0	-5.40	-3.71	723	31	99	30	0
14ed_32b_7ea	94	2	1	96	0	2	0	1	-5.42	-3.73	622	5	100	24	0
14ed_31b_7ea	93	2	1	97	0	2	0	0	-5.39	-3.72	686	22	99	24	0
14ed_16b_7ea	91	7	2	86	1	6	0	3	-5.39	-3.61	653	13	85	27	0
13ed_31b_7ea	55	3	43	95	2	2	1	0	-5.32	-3.84	705	26	84	15	0
13ed_20b_1ea	77	12	19	74	4	8	0	1	-5.44	-3.85	611	3	81	23	0
13ed_1b_9ea	6	12	11	26	81	58	0	0	-5.34	-3.64	625	6	90	31	0
13ed_1b_10ea	71	17	20	70	9	13	1	1	-5.42	-3.60	600	0	84	24	0
13ed_16b_7ea	59	13	31	81	10	6	4	3	-5.24	-3.83	747	37	87	18	0
11ed_26b_10ea	4	2	88	81	7	17	0	2	-5.17	-3.24	608	2	13	10	0
11ed_1b_7ea	72	18	20	74	6	8	2	3	-5.21	-3.23	604	1	12	23	0
11ed_1b_10ea	72	19	18	68	8	12	1	1	-5.29	-3.60	622	6	84	25	0
10ed_33b_2ea	37	1	59	97	1	2	1	1	-5.30	-3.84	712	28	85	10	0
10ed_32b_7ea	44	2	50	96	2	2	1	1	-5.38	-3.64	656	14	91	12	0
10ed_32b_2ea	48	2	47	93	2	4	1	2	-5.44	-3.82	657	14	89	14	0
10ed_31b_7ea	37	2	57	96	3	2	1	0	-5.25	-3.63	704	26	89	10	0
10ed_31b_2ea	41	2	53	94	3	4	1	2	-5.30	-3.80	707	27	94	12	0
10ed_26b_10ea	5	1	86	80	8	18	1	2	-5.06	-3.10	608	2	4	11	0
10ed_16b_7ea	43	9	41	85	13	5	5	2	-5.13	-3.41	737	34	40	14	0
10ed_16b_6ea	44	10	39	82	13	7	6	3	-5.32	-3.79	740	35	97	15	0
10ed_16b_11ea	41	11	38	81	18	7	6	3	-5.32	-3.84	733	33	82	15	0
10ed_16b_10ea	40	11	38	81	19	8	1	1	-5.25	-3.74	734	33	100	14	0

Figure S6: A molecular orbital diagram (MO) of the LSF calculated HOMO and LUMO orbital energy for the 7,906 theoretical dyes that include the iodide/triiodide redox shuttle (red dashed line) and TiO_2 semiconductor conduction bands (blue dashed line) energy levels. The theoretical dyes are separated into three groups based off of their LSF λ_{max}. A) 800-1000 nm B) 600-800 nm C) 400-600 nm



1 Experimental Supplementary Information

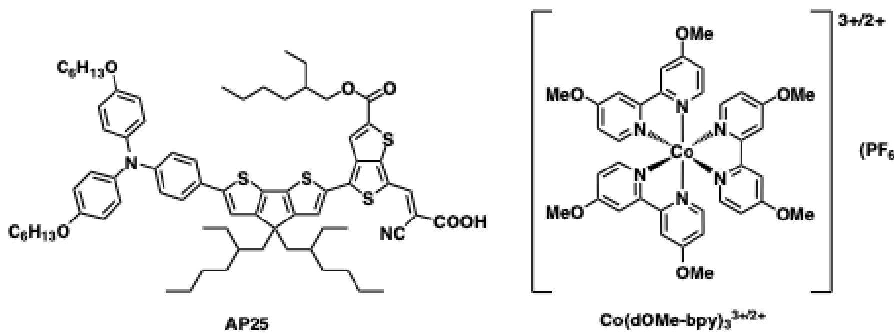
1.1 General Information

All reagents were either synthesized as previously described (see main text for reference) or purchased from commercial sources and used without further purification. Thin layer chromatography was conducted using Sorbtech glass backed 250μm Silica Gel XHL TLC plates and visualized under a UV lamp. Preparative chromatography was performed using a CombiFlash Rf + system equipped with silica gel cartridges purchased from Luknova SuperSep (particle size 50μm). NMR spectra were recorded on a Bruker Avance-400 (400MHz) spectrometer. Chemical shifts are reported in ppm using the specified NMR solvent residual protonation peak as an internal standard ($CDCl_3$ at 7.26 ppm, DMSO-d_6 at 2.50 ppm). Peaks are reported as: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sept = septet, m = multiplet, and br = broad. Coupling constants are expressed for the ^{1}H-NMR spectra in Hertz (Hz). Absorbance spectra were measured using an Avantes/AvaSpecULS2048-USB2-50 spectrometer (Pine Research part RRAVSP3) with an Avantes/AvaSpec light source (Pine Research part RRAVSP) and AvaSoft8 software program. Cyclic voltammetry measurements were recorded using a C-H Instruments Electrochemical Analyzer (CHI-600E) and were taken using a platinum counter electrode, an Ag/AgCl reference electrode, and a glassy carbon working electrode in DCM with a 0.1 M Bu_4NPF_6 electrolyte. Ferrocene was used as a reference at 0.70 V versus the normal hydrogen electrode (NHE) in DCM. HRMS spectra were obtained with a QTOF HRMS utilizing nanospray ionization with the mass analyzer set to the 200-2000 Da range. FT-IR experiments were recorded on a Bruker Alpha FT-IR spectrometer.

1.2 Device Fabrication

Fluorine doped tin oxide (FTO) coated glass was purchased from Hartford Glass. TEC 10 glass was used for the photoanodes and TEC 7 glass was used for the counter electrodes. P18 TiO_2 (particle size 18 nm, 18NR-T) and P30 TiO_2 (particle size 30 nm, 30NR-D) was purchased from Greatcell Solar and was used for the active layer (P18 used with iodine electrolyte, P30 used with cobalt electrolyte) and the scattering layer TiO_2 was purchase from Solaronix (particle size 100 nm, R/SP). Surlyn was purchased from Solaronix (25 μ m thick, Meltonix 1170). Device fabrication including glass cleaning, TiO_2 printing and sintering, preparation of the platinum counter electrodes, and Surlyn sealing was conducted in a manner previously described[95]. The photoanode was sensitized by submerging the TiO_2^- film into a dye solution containing 0.3 mM **WM3** and 6 mM CDCA in 4:1 EtOH:THF for 16 hours. After the dipping period, the photoanodes were rinsed gently with MeCN and dried under N_2flow for approximately 30 seconds before sealing with a Surlyn ring to the platinum counter electrode. Electrolyte was then added into one of the two holes of the counter electrode until the device was filled and electrolyte

Figure S7: Structure of AP25 and Co(dOMe-byp)$_3^{3+/2+}$ mentioned and/or utilized in this study.



began to exit the second hole in the counter electrode. The iodine electrolyte consisted of 0.1 M guanidinium thiocyanate, 1.0 M 1,3-Dimethylimidazolium iodide, 0.03 M iodine, 0.5 M 4-tert-Butylpyridine, and 0.1 M lithium iodide in 85:15 acetonitrile:valeonitrile. The cobalt electrolyte consisted of 0.25 M Co(dOMe-bpy)$_3$(PF$_6$)$_2$, 0.05 M Co(dOMe-bpy)$_3$(PF$_6$)$_3$, 0.25 M 4-tert-Butylpyridine, and 0.1 M LiTFSI in acetonitrile. Once the electrolyte was added, the devices were sealed with a Surlyn ring and glass cover slip and subjected to further measurements.

1.3 Device measurements

Photovoltaic characteristics were measured using a 300 W xenon lamp (Model SF300A, SCIENCETECH Inc. Class AAA) solar simulator equipped with an AM 1.5 G filter for a less than 2% spectral mismatch. Prior to each measurement, the solar simulator output was calibrated with a KG5 filtered mono-crystalline silicon NREL calibrated reference cell from ABET Technologies (Model 15150-KG5). The current density-voltage characteristic of each cell was obtained with Keithley digital source meter (Model 2400). Electrochemical impedence spectrometry was carried out using a C-H Instruments Electrochemical Analyzer (CHI-600E) under full sun irradiation. Current dynamics measurements were collected using a C-H Instruments Electrochemical Analyzer (CHI-600E) using irradiation from the solar simulator equipped with a shutter and filter wheel. The incident photon-to-current conversion efficiency was measured with an IPCE instrument manufactured by Dyenamo (DN-AE03) comprised of a 175 W xenon lamp (CERMAX, Model LX175F), monochromator (Spectral Products, Model CM110, CzernyTurner, dual-grating), filter wheel (Spectral Products, Model AB301T, fitted with filter AB3044 [440 nm high pass] and filter AB3051 [510 nm high pass]), a calibrated UV-enhanced silicon photodiode reference and Dyenamo issued software. Small modulation photovoltage transient (SMPVT) measurements were carried out with the Dyenamo toolbox (DN-AE01).

Figure S8: Cyclic voltammogram of **WM3** in DCM solution with a 0.1 M $TBAPF_6$ electrolyte referenced using Fc^+/Fc at 0.70 V vs NHE in DCM

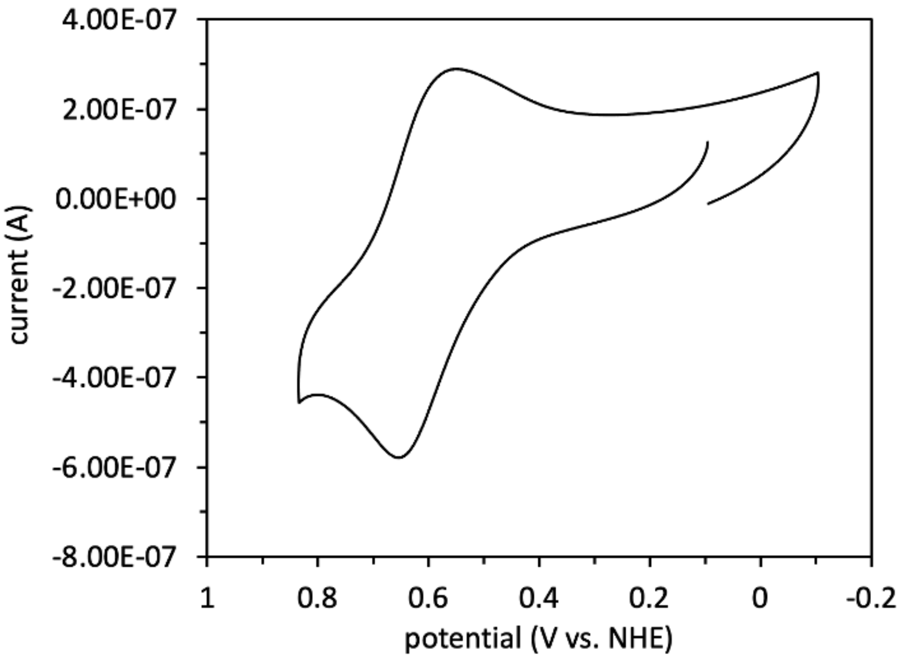
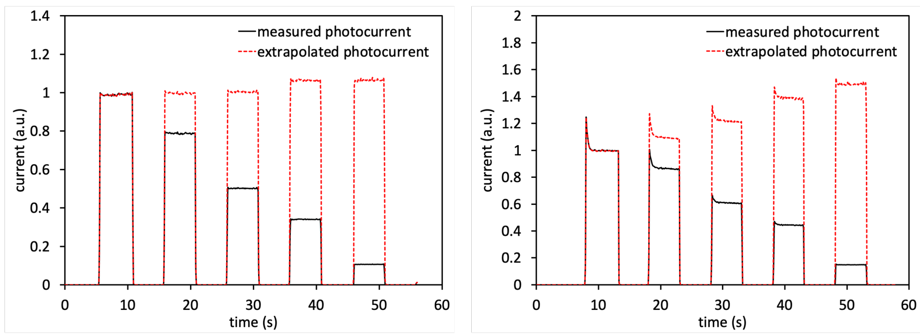


Figure S9: Current Dynamics plot of **WM3** devices with the iodine electrolyte (left) cobalt electrolyte (right).



1.4 Additionally Supplementary graphs/figures/discussion

Current dynamics plots demonstrate the amount of current generated over time at different sun intensities while the light source is shuttered on and off. The measured photocurrent is the data taken directly from the experiment, and the extrapolated photocurrent is the measured photocurrent divided by the sun intensity at each time point (1.0, 0.79, 0.50, 0.32, and 0.10 sun used herein). Iodine based devices generate an amount of photocurrent proportional to the irradiation intensity under both full sun and low light conditions demonstrated by the extrapolated photocurrent being very similar across each of the sun intensities (Figure S9, left). Further, iodine-based devices demonstrate a consistent, flat lined current production when the light is shuttered on, indicating satisfactory mass transport of the redox shuttle through the electrolyte medium to regenerate the dye. On the other hand, cobalt based devices demonstrate a photocurrent extrapolated response that is inversely proportional to the irradiation intensity (Figure S9, right). This can be seen in the extrapolated photocurrent which gradually increases as the photon flux decreases. Further, when the light is shuttered on in the cobalt devices a spike in photocurrent is observed that quickly levels off and flatlines to a consistent value. This spike indicates that there is a problem associated with mass transport of the redox shuttle through the mesoporous TiO_2, where under high photon flux conditions the redox shuttle cannot diffuse fast enough through the solution to efficiently regenerate the dye. The magnitude of this spike is observed to decrease as the photon flux decreases, indicating that as the photocurrent decreases the redox shuttle can adequately diffuse through solution to effectively regenerate the dye.

Figure S10: SMPVT plot of **WM3** devices.

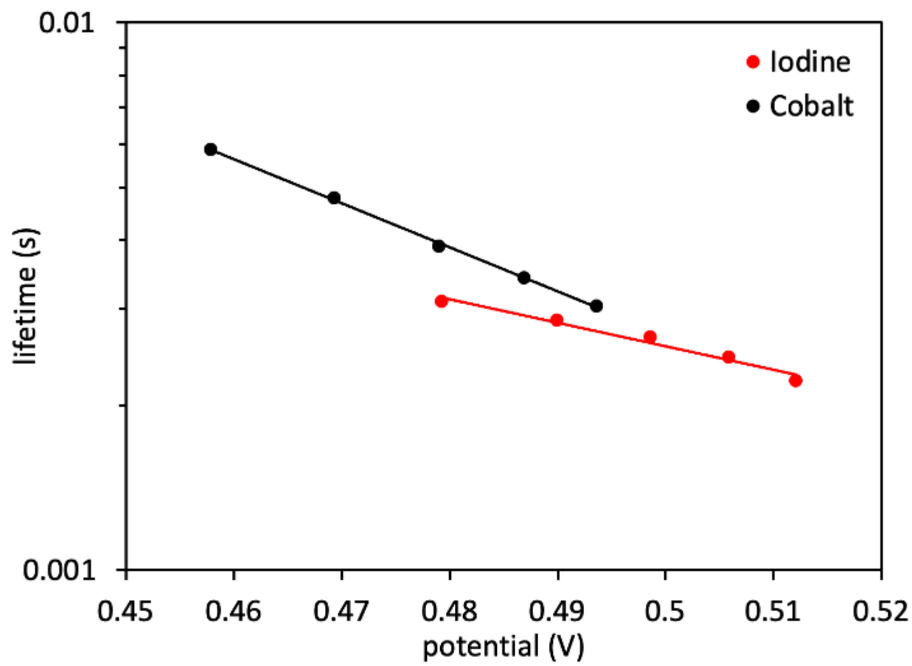


Figure S11: Nyquist plot of **WM3** devices.

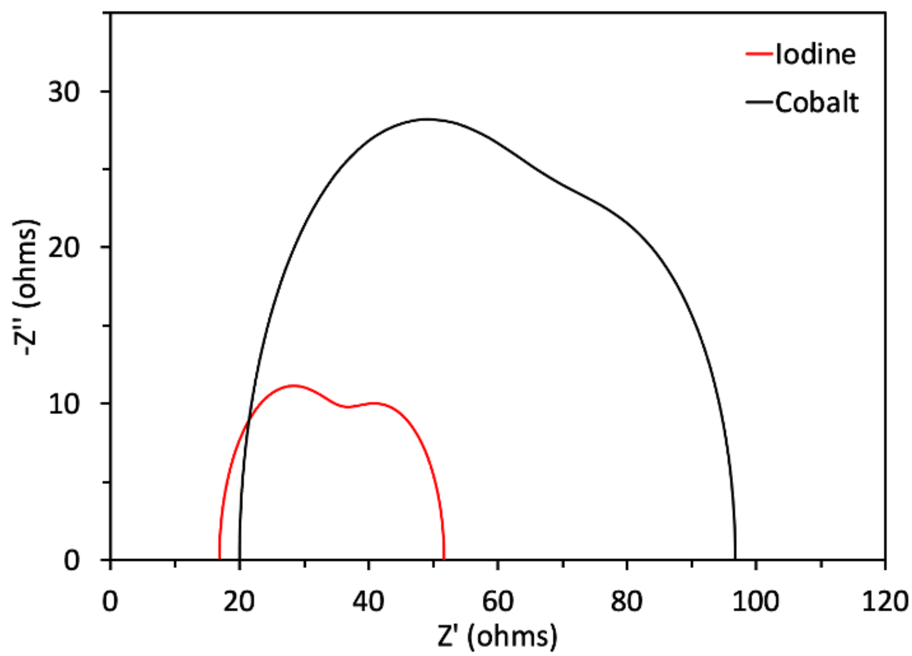
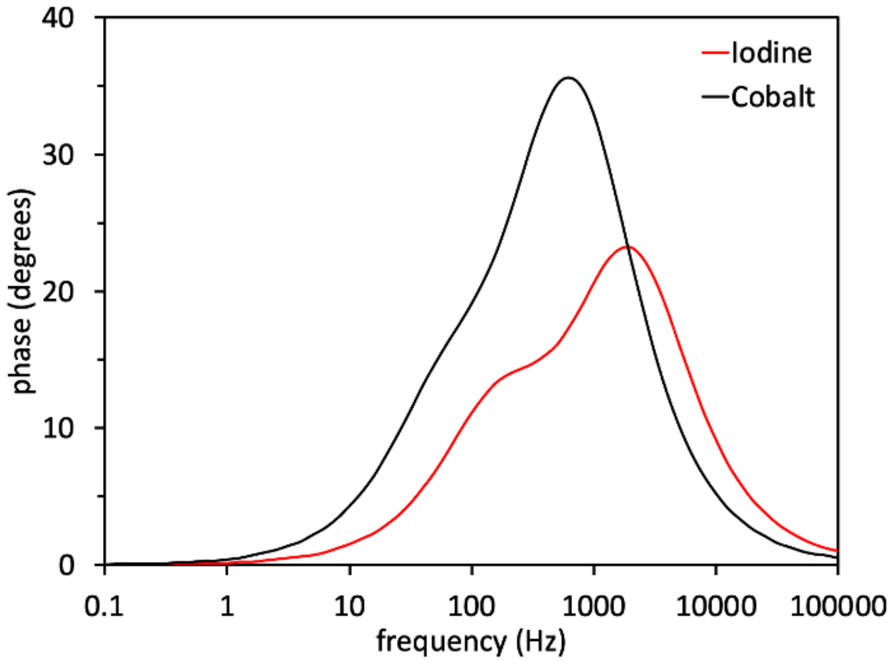
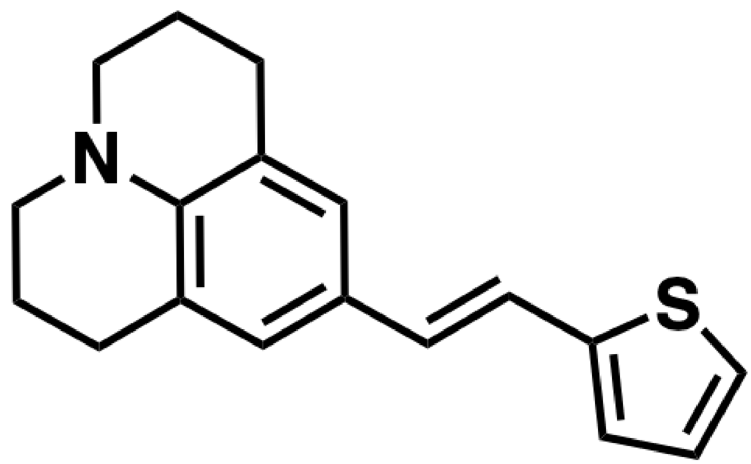


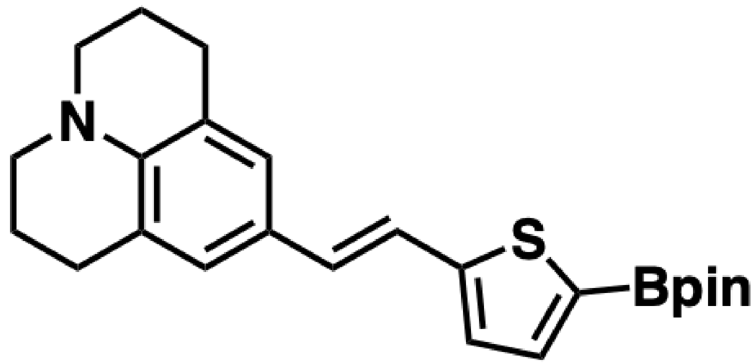
Figure S12: Bode plot of **WM3** devices



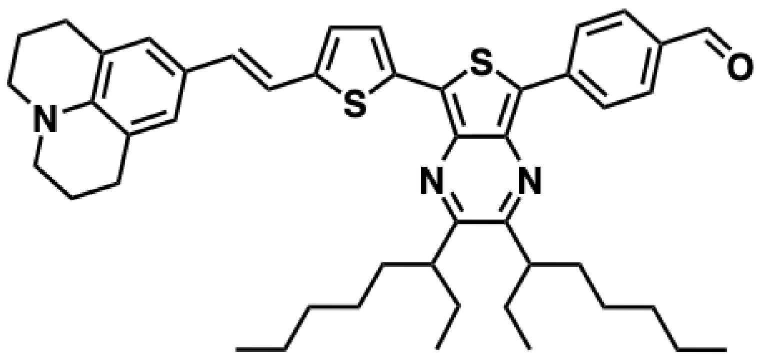
Small modulated photovoltage transient (SMPVT) measurements were conducted for **WM3** devices to observe the lifetime of electrons in TiO_2 (Figure S10). Cobalt-based devices demonstrate slightly better lifetimes than iodine-based devices, however, the two are quite close in magnitude and demonstrate no significant difference in the lifetime of electrons in TiO_2. This finding is somewhat surprising given that iodine is notorious for longer electron lifetimes in TiO_2 given its coulombically repulsive negative charge that discourages recombination.



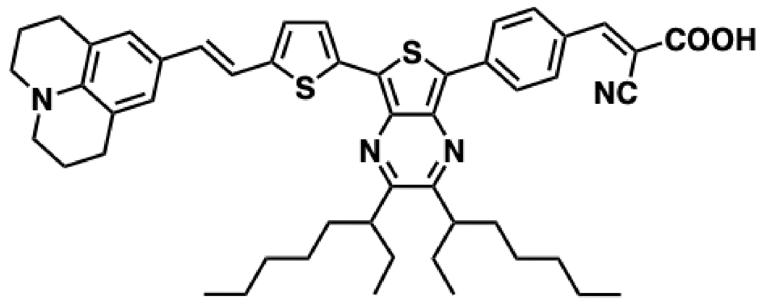
(*E*)-9-(2-(thiophen-2-yl)vinyl)-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-*ij*]quinoline (**3**): To a flame dried round bottom flask under N_2 was added 2,3,6,7-tetrahydro-1*H*,5*H*-pyrido[3,2,1-*ij*]quinoline-9-carbaldehyde (**1**, 0.304 g, 1.51 mmol) and diethyl (thiophen-2-ylmethyl)phosphonate (**2**, 0.30 mL, 1.51 mmol) in dioxane (15.1 mL, 0.1 M). KHMDS (7.6 mL, 3.8 mmol) was added dropwise to the reaction at room temperature over 10 minutes and the reaction was allowed to stir for 3 hours at room temperature. After this period there was no starting material observed via NMR. The reaction was quenched with H_2O and extracted with DCM/H_2O, the organics dried over Na_2SO_4, and concentrated to dryness to yield the crude product. The crude product was purified via silica gel chromatography using 25% DCM/Hx as an eluent to elute the pure product as a fluorescent yellow oil (0.385 g, 1.37 mmol, 91%). ^{1}H NMR (400 MHz, $CDCl_3$, Figure S11) δ 7.08 (d, J = 4.7 Hz, 1H), 6.99 - 6.95 (s, 3H), 6.93 (s, 2H), 6.77 (d, J = 16.0, 1H), 3.17 (t, J = 5.4 Hz, 4H), 2.76 (t, J = 6.4 Hz, 4H), 1.98 (t, J = 5.2 Hz, 4H) ppm. ^{13}C ^{1}H NMR (100 MHz, $CDCl_3$, Figure S12) δ 144.4, 142.7, 129.2, 127.5, 125.4, 124.3, 122.8, 121.6, 121.6, 117.0, 50.2, 27.8, 22.1. HRMS m/z calculated for $C_{18}H_{19}NS$ $[M]^+$ 281.1238, found 281.1268. IR (drop cast from DCM, cm^{-1}) 3101, 3065, 3016, 2926, 2883, 2835, 2786, 1655, 1601, 1518, 1499, 1463, 1430, 1356, 1330, 1308, 1289, 1263, 1205, 1183, 1158, 1122, 1073, 1050.



(E)-9-(2-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophen-2-yl)vinyl)-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinoline (**4**): To a flame dried round bottom flask under N_2 was added (E)-9-(2-(thiophen-2-yl)vinyl)-2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinoline (3, 0.370 g, 1.32 mmol) and THF (6.6 mL, 0.2 M). The reaction was cooled to -78^{o}C and n-BuLi (0.60 mL, 1.45 mmol) was added dropwise. The reaction was allowed to stir at -78^{o}C for 1 hour before isopropyl pinacol borate (0.54 mL, 2.63 mmol) was added dropwise to the reaction and the reaction removed from the cold bath and allowed to come to room temperature. After 3 hours at room temperature the reaction was observed to be complete via ^{1}H-NMR and was quenched via H_2O and extracted with EtOAc/H_2O 3x, the organics dried over Na_2SO_4, and concentrated to dryness to yield the crude product. The crude material was subjected to silica gel chromatography using 50% DCM/Hx to yield the product as a fluorescent yellow oil (0.174 g, 0.426 mmol, 32%) *Note that the reaction yield from the NMR appeared to be much higher (appeared quantitative) than the isolated yield and that the product was observed to be unstable on silica gel leading to the low yield. ^{1}H NMR (400 MHz, $CDCl_3$, Figure S14) δ7.50 (d, J = 3.5 Hz, 1H), 7.02 - 6.97 (m, 2H), 6.93 (s, 2H), 6.87 (d, J = 16.0 Hz, 1H), 3.18 (t, J= 5.6 Hz, 4H), 2.76 (t, J = 6.4 Hz, 4H), 1.97 (pent, J = 6.0 Hz, 4H), 1.35 (s, 12H). ^{13}C ^{1}H NMR (100 MHz, $CDCl_3$, Figure S15) δ 151.3, 143.1, 137.9, 130.8, 125.6, 125.5, 124.2, 121.5, 116.5, 84.1, 50.1, 27.8, 24.9, 22.1. HRMS m/z calculated for $C_{24}H_{30}BNO_2S$ $[M]^+$ 407.2205, found 407.2210. IR (dropcase from DCM, cm^{-1}) 3060, 3016, 2976, 2930, 2886, 2837, 2789, 1599, 1502, 1454, 1379, 1358, 1336, 1307, 1267, 1207, 1183, 1158, 1139, 1062, 1012.



(*E*)-4-(2,3-di(octan-3-yl)-7-(5-(2-(2,3,6,7-tetrahydro-1*H*, 5*H*-pyrido[3,2,1-*ij*]quinolin-9-yl)vinyl)thiophen-2-yl)thieno[3,4-b]pyrazin-5-yl)benzaldehyde (**7**): To a pressure flask under N_2 was added (*E*)-9-(2-(5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)thiophen-2-yl)vinyl)-2,3,6,7-tetrahydro-1*H*,5*H*-pyrido[3,2,1-*ij*]quinoline (**4**, 63 mg, 0.117 mmol), 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzaldehyde (**5**, 27 mg, 0.117 mmol), 5,7-dibromo-2,3-bis(2-ethylhexyl)thieno[3,4-b]pyrazine (**6**, 55 mg, 0.106 mmol), THF (2.1 mL, 0.05M), and 2.0 M K_2CO_3(aq) (0.53 mL, 0.2M). The reaction was degassed with N_2 for 15 minutes before adding $Pd(PPh_3)_4$ (6.0 mg, 0.0053 mmol), then degassed with N_2 for another for another 5 minutes, and then sealed and heated to 90^{o}C for 4 hours. After 4 hours there was no starting material remaining via TLC so the reaction was cooled to room temperature and extracted with DCM/H_2O 3x, the organics collected and dried over Na_2SO_4, and concentrated to dryness to yield the crude product. The product was purified via silica gel chromatography starting with 20% DCM/Hx and gradually increasing to 100% DCM to yield the pure product as a dark blue solid (8.1 mg, 0.011 mmol, 10%). ^{1}H NMR (400 MHz, CDCl3, Figure S16) δ 10.01 (s, 1H), 8.45 (d, J = 8.2 Hz, 2H), 7.91 (d, J = 8.4 Hz, 2H), 7.62 (d, J = 3.8 Hz, 1H), 7.00 - 6.85 (m, 5H), 3.19 (br s, 4H), 2.88 (m, 4H), 2.77 (br s, 4H), 2.30 (sept, J = 6.1 Hz, 1H), 2.18 (sept, J = 6.1 Hz, 1H), 1.99 (pent, J = 5.9 Hz, 4H), 1.59 - 1.23 (m, 16H), 0.99 (q, J = 7.9 Hz, 6H), 0.91 (q, J = 6.8 Hz, 6H) ppm. 13C 1H NMR (100 MHz, CDCl3, Figure S17) δ 191.6, 157.4, 155.8, 146.4, 143.1, 140.2, 140.0, 138.5, 134.5, 132.1, 130.3, 130.0, 129.0, 127.2, 126.1, 125.6, 125.2, 125.0, 124.5, 121.6, 116.8, 50.2, 39.7, 39.5, 37.9, 37.7, 33.1, 29.2, 27.9, 26.2, 26.1, 23.3, 22.1, 14.3, 14.3, 11.1 ppm. HRMS m/z calculated for $C_{47}H_{57}N_3OS_2$ $[M]^+$ 743.3943, found 743.3922. IR (dispersed in DCM, cm^{-1}) 3058, 3015, 2954, 2925, 2855, 2730, 1693, 1595, 1558, 1506, 1464, 1446, 1378, 1352, 1337, 1310, 1280, 1214, 1183, 1160, 1074, 1053, 1014.



(E)-2-cyano-3-(4-(2,3-di(octan-3-yl)-7-(5-((E)-2-(2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-9-yl)vinyl)thiophen-2-yl)thieno[3,4-b]pyrazin-5-yl)phenyl)acrylic acid: To a flame dried pressure flask under N_2 was added (E)-4-(2,3-di(octan-3-yl)-7-(5-(2-(2,3,6,7-tetrahydro-1H,5H-pyrido[3,2,1-ij]quinolin-9-yl)vinyl)thiophen-2-yl)thieno[3,4-b]pyrazin-5-yl)benzaldehyde (7, 8.1 mg, 0.011 mmol), cyanoacetic acid (2.7 mg, 0.032 mmol), piperidine (7.6 μL, 0.077 mmol), and $CHCl_3$ (0.2 mL, 0.05M). The reaction was sealed and heated to 95^{o}C for 45 minutes. At this time minimal starting material was observed to be remaining via TLC so the reaction was cooled to room temperature and extracted using DCM/H_2O (with 1% AcOH) 3x, the organics were collected concentrated to dryness. The crude product was then columned using 100% DCM and gradually increasing to 30% MeOH/DCM to yield the pure product as a dark green solid (8.1 mg, 0.010 mmol, 91%). ^{1}H NMR (400 MHz, DMSO-d$_6$, Figure S18) δ 8.34 (d, J = 8.3 Hz, 2H), 7.96 (d, J = 8.2 Hz, 2H), 7.91 (s, 1H), 7.63 (d, J = 3.9 Hz, 1H), 7.13 - 7.09 (m, 2H), 6.93 (s, 2H), 6.76 (d, J = 16.0 Hz, 1H), 3.16 (m, 4H), 2.89 (m, 4H), 2.69 (m, 4H), 1.88 (p, J = 5.8 Hz, 4H), 1.52 - 1.23 (m, 18H), 0.95 (q, J = 7.9 Hz, 6H), 0.86 (q, J = 6.6 Hz, 6H). HRMS m/z calculated for $C_{50}H_{57}N_4O_2S_2$ [M]$^+$ 810.4001, found 810.4020. IR (dropcast from DCM, cm^{-1}) 3351 (br), 2954, 2918, 2850, 2213, 1621, 1593, 1543, 1507, 1464, 1446, 1417, 1377, 1347, 1311, 1281, 1260, 1206, 1191, 1159, 1096, 1052, 1026.

Figure S13: ^{1}H NMR (400 MHz, $CDCl_3$) of 3

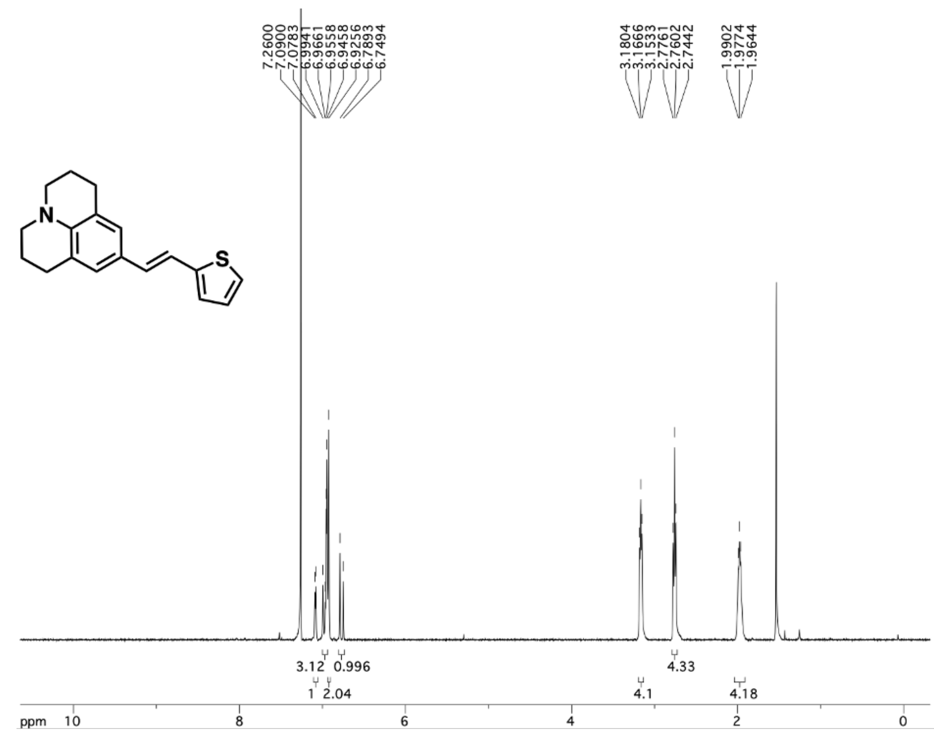


Figure S14: $^{13}C^{1}H$ (100 MHz, $CDCl_3$) of 3.

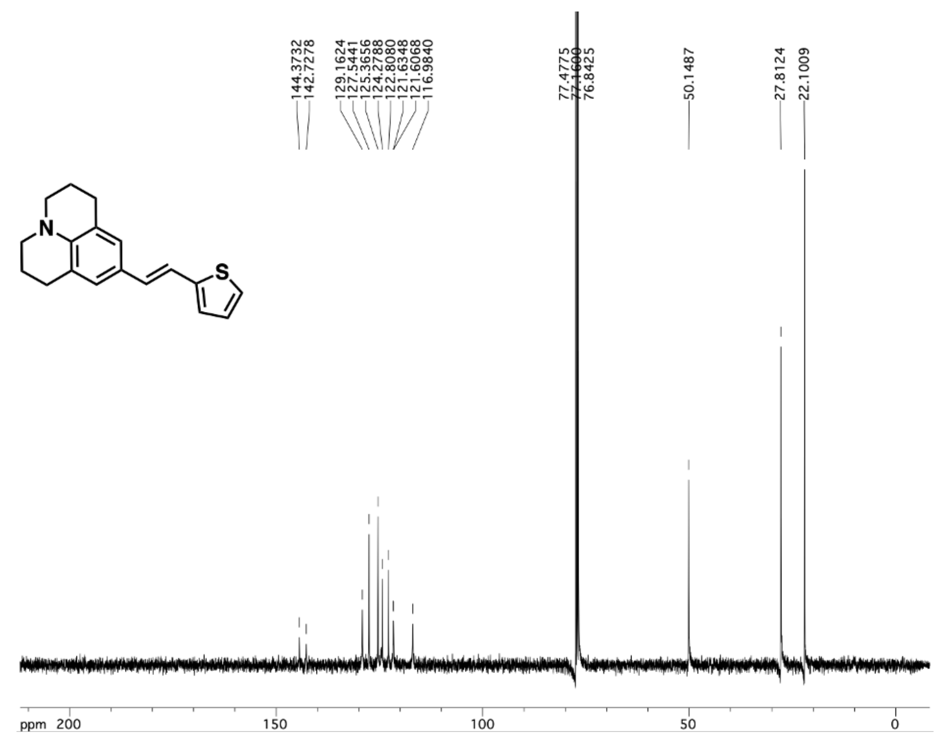


Figure S15: ^{1}H NMR (400 MHz, $CDCl_3$) of 4

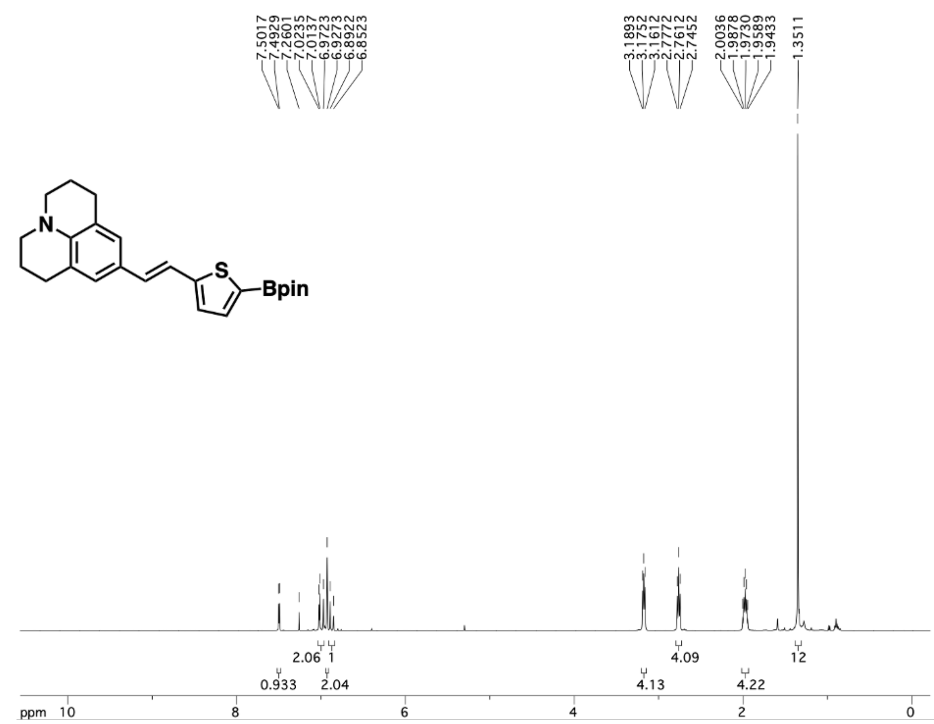


Figure S16: $^{13}C^{1}H$ (100 MHz, $CDCl_3$) of 4.

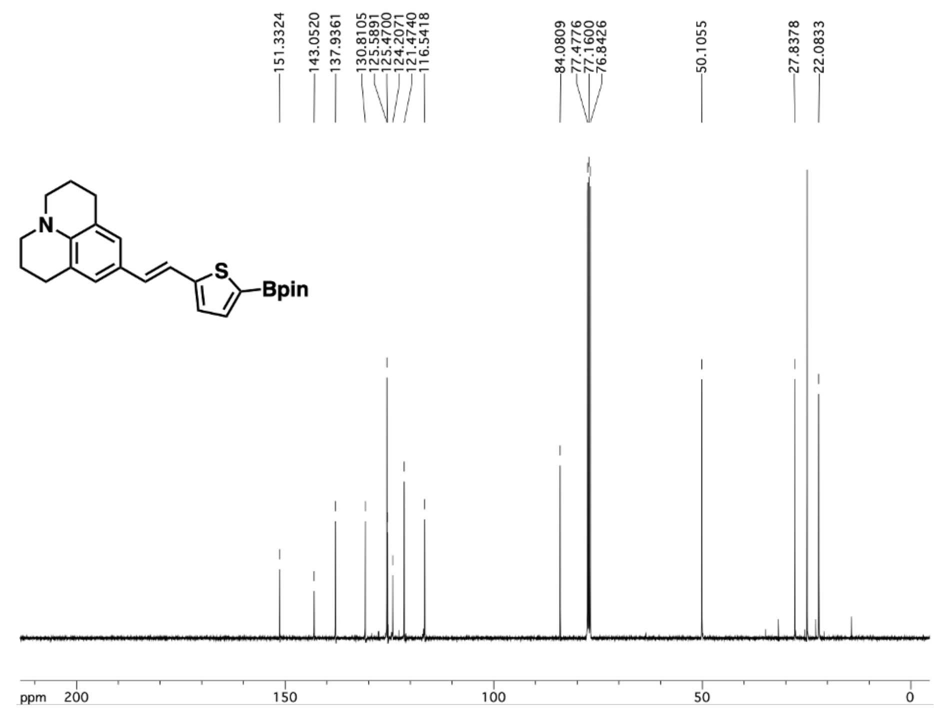


Figure S17: ^{1}H NMR (400 MHz, $CDCl_3$) of 7

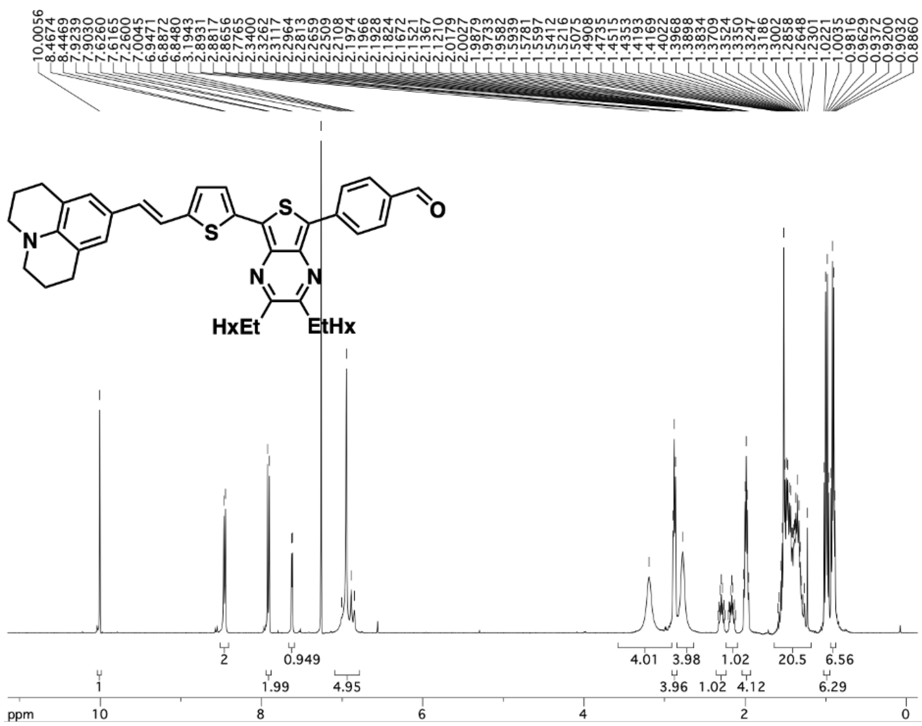


Figure S18: $^{13}C^{1}H$ (100 MHz, $CDCl_3$) of 7.

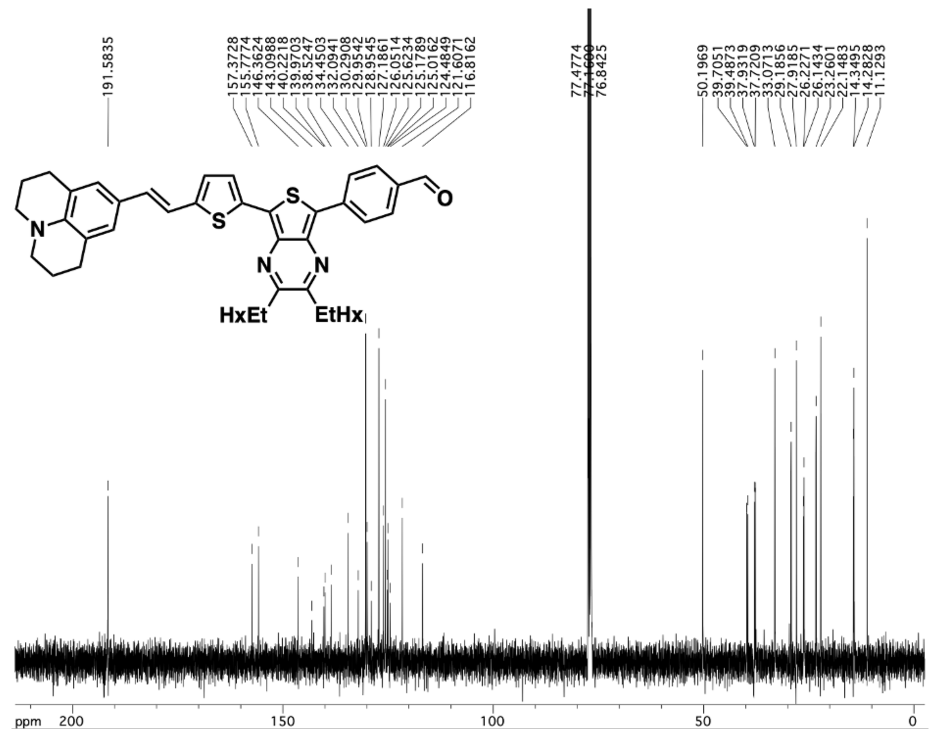


Figure S19: ^{1}H NMR (400 MHz, $CDCl_3$) of WM3

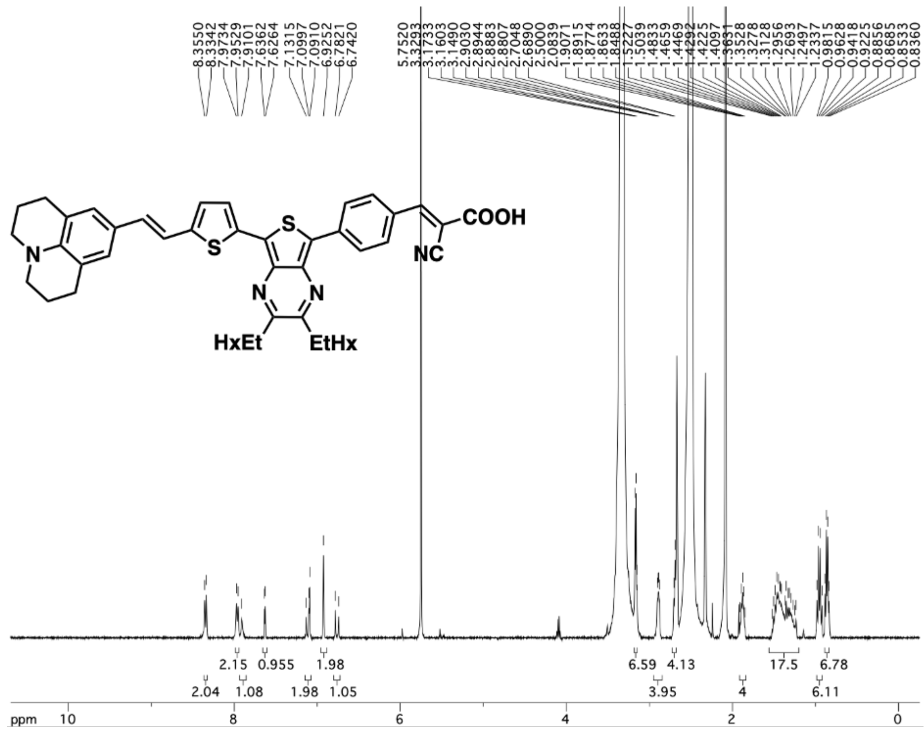
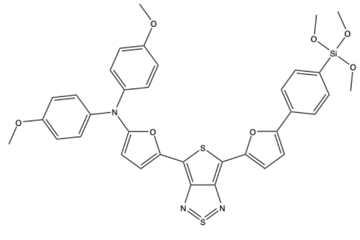
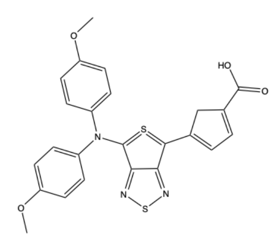


Figure S20: The theoretical dyes that are discussed for their HOMO/LUMO energy levels in the 800 to 1000 nm range from Figure S6A.

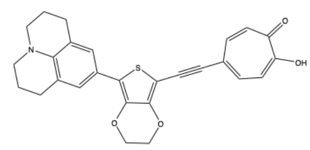


6ed_29b_7ea

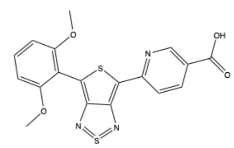


6ed_16b_5ea

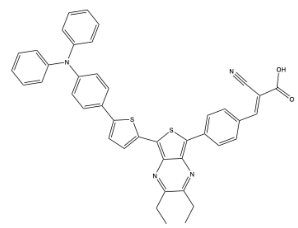
Figure S21: The theoretical dyes that are discussed for their HOMO/LUMO energy levels in the 600 to 800 nm range from Figure S6B.



22ed_11b_9ea

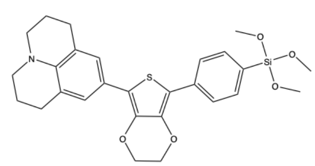


21ed_16b_2ea

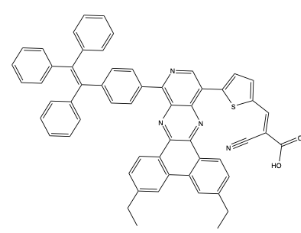


13ed_20b_1ea

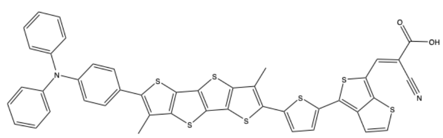
Figure S22: The theoretical dyes that are discussed for their HOMO/LUMO energy levels in the 400 to 600 nm range from Figure S6C.



22ed_11b_7ea



17ed_22b_4ea



1ed_24b_12ea

Figure S23: The theoretical dyes that are discussed for their scoring properties.

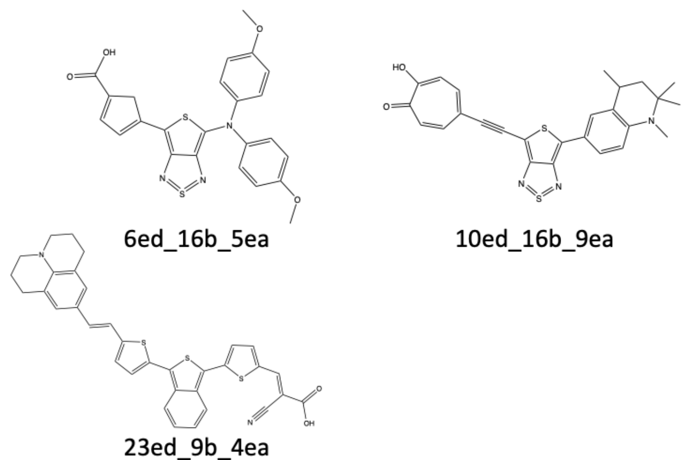


Figure S24: The geometry and selected orbitals for theoretical dye, 22ed_16b_5ea. A) HOMO and B) LUMO.

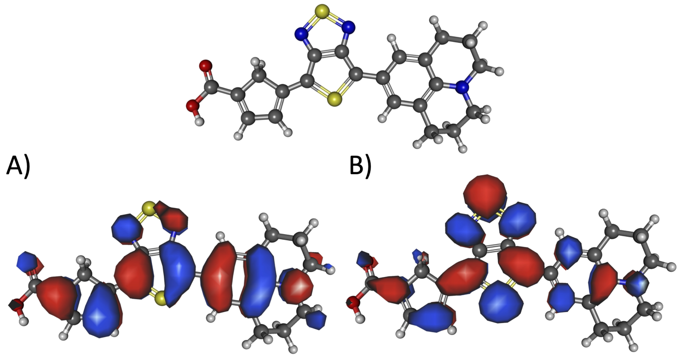


Figure S25: The geometry and selected orbitals for theoretical dye, 9ed_20b_1ea. A) HOMO and B) LUMO.