Supporting Information for:

Organic Electroactive Molecules for Li-Organic Hybrid Redox Flow Battery Application

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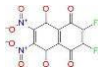
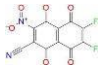
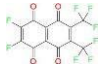
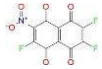
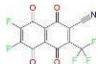
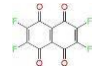
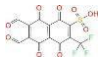
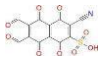
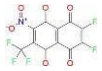
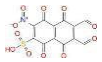
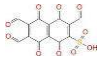
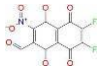
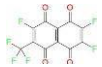
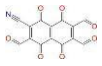
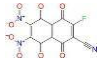
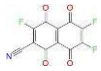
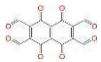
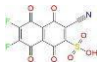
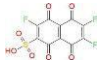
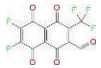
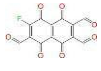
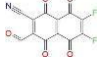
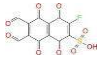
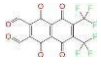
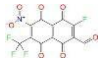
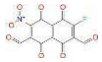
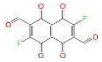
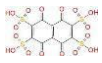
All the functional groups substituted around the functional organic molecules for tuning of their electrochemical properties. In the current supporting information page, the prepared Electroactive compound library contains thousands of molecules for analysis screened against open-source quantum semi-empirical method for overall visualization analysis and selection of electroactive organic compounds. The semi-empirical method was implemented for less computation cost and better accuracy, methods MOPAC and AM1 quantum mechanical methods using Gaussian 09 software[1], [2]. MOPAC with AM1 Open-source software which resembles an efficient and accurate quantum method was implemented for the calculation of HOMO and LUMO energy orbital energy[3] with their dipole moments. Further, the selected candidate based on homo Lumo energy as a lead descriptor selected organic material which shows promising results in the AM1 semiempirical method calculation of its electrochemical properties further analyzed by high-level quantum model density functional theory[4], [5]Here the dipole moment is the lead indicator which is proportional to the solubility factor of the organic electroactive compound.

Structure	Name	Dipole	LUMO Energy	HOMO-LUMO GAP
	DIQUINONE 322	3.938273832	-3.96	7.481
	DIQUINONE 234	2.827564063	-3.749	7.573
	DIQUINONE 224	3.661604048	-3.732	7.621
	DIQUINONE 130	1.458875474	-3.594	7.632
	DIQUINONE 177	2.872138137	-3.659	7.64
	DIQUINONE 252	4.632485514	-3.794	7.665
	DIQUINONE 88	1.349895274	-3.518	7.666
	DIQUINONE 50	1.337091916	-3.454	7.77
	DIQUINONE 157	2.379805325	-3.633	7.772
	DIQUINONE 236	3.029761335	-3.749	7.772
	DIQUINONE 15	0.002214268	-3.335	7.778
	DIQUINONE 94	1.837518033	-3.53	7.782
	DIQUINONE 36	3.365831529	-3.415	7.787
	DIQUINONE 20	2.013643424	-3.364	7.789
	DIQUINONE 189	2.778460393	-3.673	7.683
	DIQUINONE 188	4.862486837	-3.673	7.685
	DIQUINONE 60	1.589131648	-3.468	7.699
	DIQUINONE 74	2.744122712	-3.503	7.71
	DIQUINONE 100	2.289151713	-3.544	7.719
	DIQUINONE 34	2.360558118	-3.402	7.724
	DIQUINONE 101	3.634686397	-3.545	7.732
	DIQUINONE 30	1.492010801	-3.385	7.809
	DIQUINONE 118	2.987156614	-3.581	7.809
	DIQUINONE 8	2.110442046	-3.279	7.81
	DIQUINONE 81	1.88291456	-3.506	7.813
	DIQUINONE 334	3.366214668	-4.022	7.815
	DIQUINONE 174	2.202714441	-3.655	7.818
	DIQUINONE 70	4.075833612	-3.494	7.819
	DIQUINONE 42	1.365054056	-3.427	7.733
	DIQUINONE 1	2.788512659	-3.171	7.74
	DIQUINONE 57	1.919341482	-3.464	7.744
	DIQUINONE 71	2.270018334	-3.499	7.747
	DIQUINONE 286	3.282332824	-3.852	7.748
	DIQUINONE 78	3.273519987	-3.505	7.764
	DIQUINONE 119	4.034261541	-3.585	7.766
	DIQUINONE 11	1.994893245	-3.323	7.82
	DIQUINONE 3	1.278814538	-3.231	7.827
	DIQUINONE 10	2.08787903	-3.321	7.828
	DIQUINONE 61	1.708060527	-3.475	7.832
	DIQUINONE 41	2.708852516	-3.42	7.838
	DIQUINONE 5	2.09173826	-3.261	7.839
	DIQUINONE 168	2.002935523	-3.649	7.845

	DIQUINONE 179	1.980291425	-3.661	7.846
	DIQUINONE 180	2.403250825	-3.662	7.846
	DIQUINONE 97	3.593842697	-3.536	7.848
	DIQUINONE 7	0.359396307	-3.278	7.852
	DIQUINONE 317	0.066508597	-3.948	7.855
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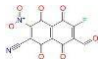
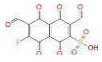
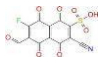
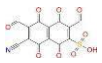
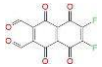
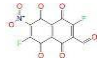
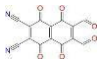
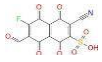
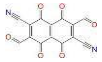
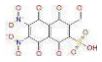
	DIQUINONE 163	2.517925117	-3.639	7.856
	DIQUINONE 23	2.749813434	-3.373	7.883
	DIQUINONE 161	3.840799137	-3.637	7.883
	DIQUINONE 22	1.807149718	-3.372	7.885
	DIQUINONE 13	1.787529417	-3.328	7.887
	DIQUINONE 249	3.762374372	-3.781	7.89
	DIQUINONE 259	0.105979531	-3.798	7.892
	DIQUINONE 51	1.947650726	-3.458	7.897
	DIQUINONE 77	3.181301405	-3.505	7.858
	DIQUINONE 19	2.410356771	-3.342	7.859
	DIQUINONE 2	2.072311941	-3.206	7.86
	DIQUINONE 129	3.042960996	-3.594	7.861
	DIQUINONE 6	1.180407278	-3.265	7.862
	DIQUINONE 103	1.948035743	-3.547	7.862
	DIQUINONE 21	2.441264225	-3.369	7.864
	DIQUINONE 54	1.595688092	-3.461	7.897
	DIQUINONE 344	3.240903657	-4.09	7.898
	DIQUINONE 38	1.906695303	-3.417	7.899
	DIQUINONE 310	5.332469833	-3.912	7.899
	DIQUINONE 16	1.222355287	-3.337	7.903
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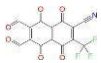
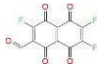
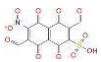
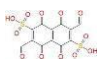
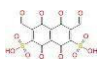
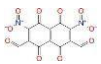
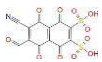
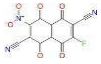
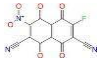
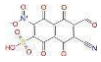
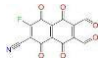
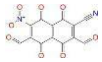
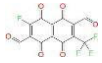
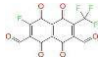
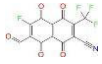
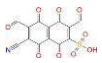
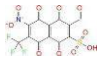
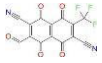
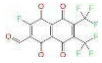
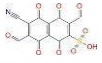
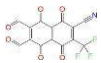
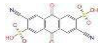
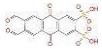
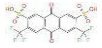
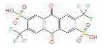
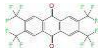
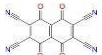
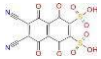
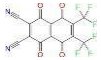
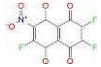
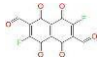
	DIQUINONE 35	0.772300021	-3.415	7.864
	DIQUINONE 4	0.950589234	-3.257	7.868
	DIQUINONE 195	3.044112342	-3.691	7.87
	DIQUINONE 123	0.927741218	-3.589	7.875
	DIQUINONE 92	4.376242527	-3.529	7.879
	DIQUINONE 269	5.429049734	-3.812	7.88
	DIQUINONE 304	3.327055782	-3.894	7.881
	DIQUINONE 138	1.63373917	-3.605	7.906
	DIQUINONE 271	2.819717991	-3.818	7.907
	DIQUINONE 272	1.86670534	-3.818	7.908
	DIQUINONE 351	0.030532334	-4.45	7.908
	DIQUINONE 225	2.812166924	-3.733	7.915
	DIQUINONE 31	3.586908926	-3.392	7.916
	DIQUINONE 128	1.609538982	-3.594	7.916

	DIQUINONE 67	1.454054632	-3.488	7.917
	DIQUINONE 9	1.966493723	-3.281	7.919
	DIQUINONE 120	4.143589991	-3.586	7.919
	DIQUINONE 313	3.537684239	-3.922	7.925
	DIQUINONE 12	1.668707715	-3.324	7.928
	DIQUINONE 14	2.507690824	-3.334	7.928
	DIQUINONE 49	1.008632991	-3.45	7.931
	DIQUINONE 187	1.208291784	-3.67	7.932
	DIQUINONE 281	2.60218899	-3.836	7.932
	DIQUINONE 48	0.677684322	-3.447	7.937
	DIQUINONE 280	2.49515742	-3.834	7.938
	DIQUINONE 122	2.238331344	-3.587	7.939
	DIQUINONE 59	0.931374852	-3.467	7.942
	DIQUINONE 43	1.400931129	-3.434	7.946
	DIQUINONE 244	1.838979743	-3.765	7.949

Structure	Name	Dipole	LUMO Energy	HOMO LUMO GAP
	QUINONE_TYPE_2,TRI FLUORINE,SH	3.324168638	-2.019	7.29
	QUINONE TYPE 2,NITRO,SH	4.834926733	-2.193	7.302
	QUINONE TYPE 2,PHOSPHONYL,SH	3.682104376	-2.124	7.37
	QUINONE TYPE 2,SULPHONYL,SH	4.099414198	-2.18	7.38
	QUINONE_TYPE_2,NITRO,2 AMINE	3.705061316	-2.082	7.456
	QUINONE TYPE 2,PHOSPHONYL,ETHELENE	2.31978164	-2.055	7.948
	QUINONE TYPE 2,SULPHONYL,ETHELENE	2.786568873	-2.144	7.95
	QUINONE TYPE 2,NITRO,ETHELENE	4.111365884	-2.163	7.988
	QUINONE TYPE 2,NITRO,OCH3	5.461399332	-2.133	8.12
	QUINONE TYPE 2,CYANIDE,ETHYLENE	2.182079406	-2.01	8.136
	QUINONE TYPE 2,SULPHONYL,ETHYLENE	3.964363984	-2.211	8.148
	QUINONE TYPE 2,PHOSPHONYL,OCH3	4.894258947	-2.015	8.171
	QUINONE TYPE 2,PHOSPHONYL,ETHYLENE	3.348085777	-2.1	8.179
	QUINONE_TYPE_2,TRI FLUORINE,ETHYLENE	2.358095125	-2.035	8.212
	QUINONE_TYPE_2,SULPHONYL,2 AMINE	3.800488238	-2.083	8.218
	QUINONE TYPE 2,NITRO,OH	5.37903734	-2.213	8.219
	QUINONE TYPE 2,SULPHONYL,OCH3	6.012512684	-2.107	8.234
	QUINONE TYPE 2,NITRO,ETHYLENE	3.781419678	-2.213	8.251
	QUINONE TYPE 2,PHOSPHONYL,OH	4.509207957	-2.085	8.256
	QUINONE_TYPE_2,PHOSPHONYL,2 AMINE	3.710851509	-2.045	8.264
	QUINONE TYPE 2,SULPHONYL,OH	5.663699714	-2.176	8.31

	QUINONE TYPE 2,FORMYL,FLUORINE	2.895832389	-2.029	8.347
	QUINONE TYPE 2,CYANIDE,CHOLRINE	2.635248736	-2.092	8.358
	QUINONE TYPE 2,CYANIDE,FLUORINE	2.993776821	-2.12	8.388
	QUINONE TYPE 2,SULPHONYL,CHOLRINE	3.111499196	-2.281	8.389
	QUINONE TYPE 2,FORMYL,CHOLRINE	2.049630421	-2.01	8.393
	QUINONE TYPE 2,PHOSPHONYL,CHOLRINE	3.097164512	-2.231	8.409
	QUINONE TYPE 2,SULPHONYL,FLUORINE	3.76140572	-2.322	8.43
	QUINONE TYPE 2,PHOSPHONYL,FLUORINE	3.217748353	-2.272	8.432
	QUINONE_TYPE_2_CARBOXYLIC ACID,CHLORINE	1.641958916	-1.993	8.435
	QUINONE TYPE 2,NITRO,FLUORINE	4.896418636	-2.422	8.438
	QUINONE_TYPE_2,TRI FLUORINE,CHOLRINE	2.722350746	-2.122	8.438
	QUINONE_TYPE_2_CARBOXYLIC ACID,FLUORINE	1.936133591	-2.019	8.471
	QUINONE_TYPE_2,TRI FLUORINE,FLUORINE	3.080171894	-2.156	8.484
	QUINONE TYPE 2,NITRO,CHOLRINE	4.305588086	-2.302	8.49
	QUINONE TYPE 2,CYANIDE,SULPHONYL	4.236768843	-2.522	8.507
	QUINONE TYPE 2,PHOSPHONYL,SILICATE	5.259024528	-2.028	8.533
	QUINONE TYPE 2,CYANIDE,PHOSPHONYL	3.040985558	-2.408	8.538
	QUINONE TYPE 2,CYANIDE,SILICATE	1.969828221	-2.033	8.544
	QUINONE TYPE 2,CYANIDE,CYANIDE	4.1048709	-2.318	8.549
	QUINONE TYPE 2,CYANIDE,FORMYL	2.488226348	-2.249	8.56
	QUINONE TYPE 2,FORMYL,SULPHONYL	2.664138091	-2.394	8.584
	QUINONE_TYPE_2_ALKENYL KETONE,FORMYL	3.349851234	-2.129	8.593
	QUINONE_TYPE_2_CARBOXYLIC ACID,FORMYL	2.850281797	-2.181	8.601
	QUINONE TYPE 2,FORMYL,FORMYL	1.655630558	-2.121	8.606
	QUINONE TYPE 2,SULPHONYL,SILICATE	2.104693341	-2.228	8.619
	QUINONE_TYPE_2 ,CYANIDE,TRI FLUORINE	4.173891866	-2.355	8.628
	QUINONE_TYPE_2_CARBOXYLIC ACID, ALKENYL ALKENE	2.867855998	-2.165	8.632
	QUINONE_TYPE_2_CARBOXYLIC ACID, ALKENYL ALKENE	3.545790321	-2.088	8.639
	QUINONE_TYPE_2_CARBOXYLIC ACID,ALKENYL ACID	3.147473814	-2.217	8.641
	QUINONE TYPE 2,FORMYL,PHOSPHONYL	3.938112825	-2.297	8.643
	QUINONE_TYPE_2_ALKENYL KETONE,PHOSPHONYL	3.070028355	-2.177	8.643
	QUINONE_TYPE_2_ALKENYL KETONE,SULPHONYL	5.368950057	-2.333	8.649
	QUINONE_TYPE_2_ALKENYL ALKENE,SULPHONYL	5.179256328	-2.395	8.659
	QUINONE TYPE2,NITRO,FORMYL	4.390331514	-2.501	8.664
	QUINONE_TYPE_2_CARBOXYLIC ACID,SILICATE	1.483672482	-2.011	8.674
	QUINONE_TYPE_2_CARBOXYLIC ACID,SULPHONYL	4.983317699	-2.46	8.675
	QUINONE_TYPE_2_CARBOXYLIC ACID,ALKENYL KETONE	3.052628708	-2.048	8.68
	QUINONE TYPE2,NITRO,SILICATE	3.231249888	-2.396	8.684
	QUINONE_TYPE_2 ,FORMYL,TRI FLUORINE	2.541831989	-2.275	8.691
	QUINONE TYPE 2,NITRO,CYANIDE	5.609005752	-2.535	8.692
	QUINONE_TYPE_2_ALKENYL KETONE,PHOSPHONYL	3.05444362	-2.261	8.702
	QUINONE_TYPE_2_CARBOXYLIC ACID,PHOSPHONYL	3.498716378	-2.326	8.715

	QUINONE_TYPE_2 ,NITRO,METHYL KETONE	5.163915055	-2.393	8.718
	QUINONE TYPE 2,SULPHONYL,PHOSPHONYL	5.733920438	-2.369	8.718
	QUINONE TYPE 2,NITRO,SULPHONYL	5.536823056	-2.794	8.738
	QUINONE TYPE 2,SULPHONYL,SULPHONYL	5.327804815	-2.624	8.741
	QUINONE_TYP E_2_M ETH YL KETONE,TRI FLUORINE	3.487550614	-2.115	8.751
	QUINONE_TYPE_2,NITRO,METHYL EASTER	4.128226476	-2.471	8.763
	QUINONE_TYP E_2_ TRI FLUORINE,SULPH ONYL	4.625567782	-2.505	8.773
	QUINONE_TYPE_2 ,TRI FLUORINE,SILICATE	2.033503683	-2.086	8.775
	QUINONE_TYPE_2,NITRO,CARBOXYLIC ACID	4.372730802	-2.53	8.779
	QUINONE_TYP E_2_M ETH YL KETONE,METH YL KETONE	2.855533446	-2.012	8.788
	QUINONE TYPE 2,PHOSPH ONYL,PH OSPH ONYL	5.140851396	-2.499	8.79
	QUINONE TYPE 2,NITRO,PHOSPHON YL	6.04384111	-2.611	8.799
	QUINONE_TYPE_2_METHYL ESTER,CARBOXYLIC ACID	2.737704774	-2.061	8.802
	QUINONE_TYP E_2_ TRI FLUORINE,PH OSPH ONYL	4.051515431	-2.448	8.804
	QUINONE_TYP E_2_M ETH YL KETONE,TRI FLUORINE	2.891675383	-2.191	8.811
	QUINONE_TYP E_2_CARB OXYLIC ACID,METHYL ESTER	2.740384037	-2.111	8.818
	QUINONE_TYP E_2_CARB OXYLIC ACID,TRI FLUORINE	3.201817449	-2.246	8.834
	QUINONE TYPE 2,NITRO,NITRO	7.022669993	-2.849	8.843
	QUINONE_TYP E_2_ TRI FLUORINE,TRI FLUORINE	4.248451942	-2.387	8.873
	QUINONE_TYPE_2,NITRO,TRI FLUORINE	5.680824695	-2.565	8.92

STRUCTURE	NAME	Dipole	LUMO Energy	E (red) in mili volts multi e
	COMPOUND 01	7.015251988	-2.796	120.7547513
	COMPOUND 02	4.858774771	-2.307	119.468651
	COMPOUND 03	0.562743809	-2.639	110.6736491
	COMPOUND 04	2.206734728	-2.643	111.0215844
	COMPOUND 05	0.00011463	-2.823	110.5478219
	COMPOUND 06	4.939189827	-2.376	112.5122636
	COMPOUND 07	4.360454815	-2.353	109.3228148
	COMPOUND 08	2.215641371	-2.596	115.4679904
	COMPOUND 09	4.590214072	-2.329	113.2159603
	COMPOUND 10	0.006091204	-3.84	115.8148652
	COMPOUND 11	4.488140952	-2.472	116.2908373
	COMPOUND 12	3.367416239	-3.52	112.6330127
	COMPOUND 13	5.142139388	-2.097	218.8446006
	COMPOUND 14	0.000889789	-2.696	207.2443294
	COMPOUND 15	0.002092637	-4.069	222.8555606
	COMPOUND 16	1.712359713	-2.896	215.2917203
	COMPOUND 17	4.15935607	-3.497	207.372564
	COMPOUND 18	0.007678396	-3.551	207.1589299
	COMPOUND 19	0.002164481	-3.738	212.4137221
	COMPOUND 20	2.07659277	-3.985	215.8770243
	COMPOUND 21	0.00025318	-3.599	232.3364291

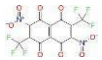
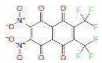
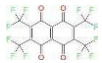
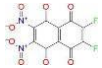
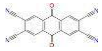
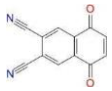
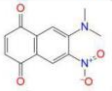
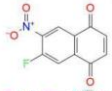
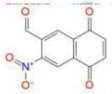
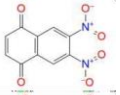
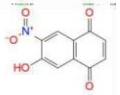
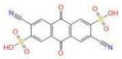
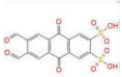
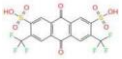
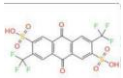
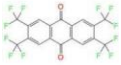
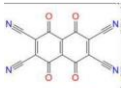
	COMPOUND 22	0.375916478	-3.669	232.3669038
	COMPOUND 23	1.787364479	-3.435	213.7979021
	COMPOUND 24	2.745144589	-3.539	222.2178933
	COMPOUND 25	3.454710479	-3.808	212.7426531
	COMPOUND 26	5.890995429	-3.494	218.0747093
	COMPOUND 27	0.864850882	-3.474	210.0972559
	COMPOUND 28	3.060026832	-2.68	125.3372446

Table 01. Contain all the quinone & teraone derivatives' electrochemical properties calculated by Mopac opensource semiempirical method used to calculate the dipole moment and Homo Lumo energy measured by AM1 semi-empirical method present in the gaussian 09 software package.

STRUCTURE	COMPOUND	Semi-Empirical Method	Mol. MW	dipole	LUMO Energy	HOMO-LUMO GAP	QM Method	QM Basis	LUMO	$\Delta G^{\circ}_{(red,\ sol.)}$ (Kcal/Mol.)	E° VS SHE Reduction In Millivolts
	COMPOUND 01	PM3	208.176	7.625	-2.329	8.517	DFT(b3lyp-d3)	6-31g++**	-0.23432	-2.784604564	120.7547513
	COMPOUND 02	PM3	251.164	6.502	-2.353	8.629	DFT(b3lyp-d3)	6-31g++**	-0.23376	- 2.75494709	119.468651
	COMPOUND 03	PM3	246.222	4.477	-2.091	7.774	DFT(b3lyp-d3)	6-31g++**	-0.23086	-2.552134349	110.6736491
	COMPOUND 04	PM3	221.144	6.169	-2.376	8.651	DFT(b3lyp-d3)	6-31g++**	-0.22954	-2.560157735	111.0215844
	COMPOUND 05	PM3	231.164	6.118	-2.307	8.815	DFT(b3lyp-d3)	6-31g++**	-0.22885	-2.549232773	110.5478219
	COMPOUND 06	PM3	248.151	8.777	-2.796	8.921	DFT(b3lyp-d3)	6-31g++**	-0.22127	-2.594532798	112.5122636
	COMPOUND 07	PM3	219.153	6.561	-2.097	8.376	DFT(b3lyp-d3)	6-31g++**	-0.22116	-2.52098411	109.3228148
	COMPOUND 08	PM3	418.352	2.878	-2.596	8.518	DFT(b3lyp-d3)	6-31g++**	-0.21992	-2.662691859	115.4679904
	COMPOUND 09	PM3	424.353	4.796	-2.472	8.458	DFT(b3lyp-d3)	6-31g++**	-0.21823	-2.610760044	113.2159603
	COMPOUND 10	PM3	504.329	2.278	-2.643	8.8	DFT(b3lyp-d3)	6-31g++**	-0.21706	-2.670690791	115.8148652
	COMPOUND 11	PM3	504.329	1.193	-2.639	8.811	DFT(b3lyp-d3)	6-31g++**	-0.21471	-2.681666709	116.2908373
	COMPOUND 12	PM3	480.209	0	-2.823	8.768	DFT(b3lyp-d3)	6-31g++**	-0.21309	-2.597317272	112.6330127
	COMPOUND 13	PM3	288.178	0.001	-3.599	8.194	DFT(b3lyp-d3)	6-31g++**	-0.21156	-5.046556491	218.8446006
	COMPOUND 14	PM3	274.14	3.978	-3.435	8.145	DFT(b3lyp-d3)	6-31g++**	-0.20939	-4.779054235	207.2443294

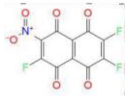
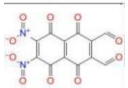
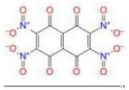
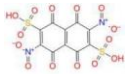
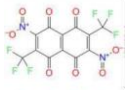
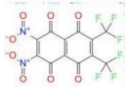
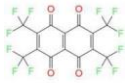
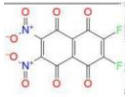
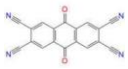
	COMPOUND 15	PM3	398.275	1.874	-3.474	7.928	DFT(b3lyp-d3)	6-31g++**	-0.19696	-5.139049228	222.8555606
	COMPOUND 16	PM3	374.155	2.13	-3.669	8.147	DFT(b3lyp-d3)	6-31g++**	-0.17838	-4.964627069	215.2917203
	COMPOUND 17	PM3	287.108	3.441	-3.539	8.109	DFT(b3lyp-d3)	6-31g++**	-0.17695	-4.782011327	207.372564
	COMPOUND 18	PM3	280.141	2.121	-2.896	8.286	DFT(b3lyp-d3)	6-31g++**	-0.1698	-4.777084924	207.1589299
	COMPOUND 19	PM3	334.155	8.131	-3.494	7.936	DFT(b3lyp-d3)	6-31g++**	-0.16919	-4.898260431	212.4137221
	COMPOUND 20	PM3	368.13	0.003	-4.069	8.341	DFT(b3lyp-d3)	6-31g++**	-0.16834	-4.97812418	215.8770243
	COMPOUND 21	PM3	438.251	5.983	-3.497	8.282	DFT(b3lyp-d3)	6-31g++**	-0.16565	-5.357678056	232.3364291
	COMPOUND 22	PM3	438.251	0.008	-3.551	8.257	DFT(b3lyp-d3)	6-31g++**	-0.16515	-5.358380801	232.3669038
	COMPOUND 23	PM3	414.131	0.007	-3.84	8.468	DFT(b3lyp-d3)	6-31g++**	-0.16326	-4.930179622	213.7979021
	COMPOUND 24	PM3	449.192	4.929	-3.52	8.379	DFT(b3lyp-d3)	6-31g++**	-0.16176	-5.12434462	222.2178933
	COMPOUND 25	PM3	414.131	2.478	-3.985	8.244	DFT(b3lyp-d3)	6-31g++**	-0.16081	-4.905845581	212.7426531
	COMPOUND 26	PM3	460.132	0.004	-3.738	8.251	DFT(b3lyp-d3)	6-31g++**	-0.15675	-5.028802797	218.0747093
	COMPOUND 27	PM3	314.115	4.309	-3.808	7.959	DFT(b3lyp-d3)	6-31g++**	-0.14858	-4.844842722	210.0972559
	COMPOUND 28	PM3	308.255	0.001	-2.696	8.356	DFT(b3lyp-d3)	6-31g++**	-0.14414	-2.890276861	125.3372446

Table 02: Electrochemical properties of the above organic functional material computed using Gaussian 09 software with B2LYP-D3 DFT function and 6-31++G (d, p) basis set and PM3 semiempirical method in Gaussian 09 software.

[1] R. Sundararaman, K. Letchworth-Weaver, K. A. Schwarz, D. Gunceler, Y. Ozhabes, and T. A. Arias, "JDFTx: Software for joint density-functional theory," *SoftwareX*, vol. 6, pp. 278–284, Jan. 2017, doi: 10.1016/J.SOFTX.2017.10.006.

[2] M. H. Baik and R. A. Friesner, "Computing redox potentials in solution: Density functional theory as a tool for rational design of redox agents," *Journal of Physical Chemistry A*, vol. 106, no. 32, pp. 7407–7412, Aug. 2002, doi: 10.1021/JP025853N/SUPPL_FILE/JP025853N_S.PDF.

[3] A. R. Matamala and A. A. Alarcon, "A simple model for the calculation of HOMO and LUMO energy levels of benzocatafusenes," *Int J Quantum Chem*, vol. 112, no. 5, pp. 1316–1322, Mar. 2012, doi: 10.1002/QUA.23135.

[4] H. Neugebauer, F. Bohle, M. Bursch, A. Hansen, and S. Grimme, "Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods," *Journal of Physical Chemistry A*, vol. 124, no. 35, pp. 7166–7176, Sep. 2020, doi: 10.1021/ACS.JPCA.0C05052/SUPPL_FILE/JP0C05052_SI_003.PDF.

[5] J. C. Panitz, T. Lippert, J. Stebani, O. Nuyken, and A. Wokaun, "AM1 and PM3 semiempirical calculations on 1-aryl-3,3-diethyltriazenes. Correlation of bond orders with rotational barriers and quantum yields of photolysis," *Journal of Physical Chemistry*, vol. 97, no. 20, pp. 5246–5253, 1993, doi: 10.1021/J100122A013/ASSET/J100122A013.FP.PNG_V03.