Supplementary Information

Exploration of Linear and Third-order Nonlinear Optical Properties for Donor-π linker-Acceptor Chromophores Derived from ATT-2 Based Non-fullerene Molecule

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Table S1: Cartesian coordinates of **ATTR1.**

Atom	X-axis	Y-axis	Z-axis
C	-0.32841	-1.38659	0.071583
C	0.987857	-0.97567	0.071205
C	1.314433	0.399344	0.072734
C	0.328379	1.386507	0.071646
C	-0.98788	0.975588	0.07121
C	-1.31446	-0.39943	0.072669
H	-0.59179	-2.44215	0.071861
H	0.591763	2.442065	0.071957
C	-2.75294	-0.47503	0.076341
C	-3.3118	0.784515	0.073734
C	-4.70572	0.771678	0.083639
H	-5.33353	1.657391	0.093914
C	3.311776	-0.7846	0.073786
C	4.705695	-0.77175	0.083693
C	5.222884	0.513981	0.09422
H	5.333518	-1.65745	0.093934
S	-3.9363	-1.71879	0.088532
S	3.936247	1.718716	0.088625
C	2.752906	0.474947	0.076424

C	-5.22292	-0.51404	0.09416
C	-2.23735	1.841134	0.071518
C	2.23732	-1.84122	0.071514
C	-8.5806	-2.13978	0.228462
C	-7.17471	-2.14801	0.256742
C	-6.59723	-0.89675	0.103412
S	-7.82843	0.323573	-0.09209
C	9.132428	0.853809	0.048027
C	8.580556	2.139758	0.228311
C	7.174667	2.147965	0.256769
S	7.828384	-0.3236	-0.09223
C	-9.13248	-0.85381	0.048323
C	6.597179	0.896704	0.103452
C	-10.5141	-0.66275	-0.00671
C	10.51402	0.662733	-0.00696
C	11.33509	-0.43662	-0.16559
H	11.02439	1.614006	0.105084
C	12.78172	-0.43934	-0.20011
C	13.64621	0.631379	-0.0948
C	13.40661	-4.60411	-0.7195
C	14.5477	-3.81216	-0.64905
C	14.47201	-2.43232	-0.47902
C	13.21618	-1.84364	-0.37936
C	12.0805	-2.6555	-0.45255
C	12.1485	-4.02234	-0.62011
H	15.38704	-1.85801	-0.42875
H	11.23745	-4.61052	-0.67091
C	10.87417	-1.81918	-0.32631
C	15.05957	0.504365	-0.14774
N	16.21402	0.453526	-0.18501
C	13.22982	1.978088	0.077059
N	12.92553	3.085118	0.218368
O	9.725823	-2.22136	-0.35332
H	-11.0245	-1.61401	0.105355
C	-11.3351	0.436628	-0.16536
C	-10.8741	1.81918	-0.3259
C	-12.7817	0.439425	-0.20004
C	-13.6463	-0.63123	-0.09487
O	-9.72569	2.221298	-0.35265
C	-13.2161	1.843739	-0.37942
C	-12.0803	2.655549	-0.45245
C	-12.1483	4.022385	-0.62002
C	-13.4064	4.604189	-0.71959
C	-14.5475	3.812288	-0.64928
C	-14.4719	2.432447	-0.47922
H	-11.2372	4.610566	-0.67069
H	-15.3869	1.858128	-0.42901
C	-13.23	-1.97794	0.077252

N	-12.9257	-3.08495	0.218797
C	-15.0596	-0.50418	-0.1483
N	-16.214	-0.4533	-0.18598
C	2.311373	-2.70961	1.327119
H	1.484149	-3.42744	1.347644
H	3.250703	-3.27365	1.345095
H	2.259441	-2.09625	2.232511
C	2.313412	-2.70842	-1.18471
H	1.486173	-3.42618	-1.20733
H	2.263115	-2.09424	-2.08963
H	3.252873	-3.2723	-1.20144
C	-2.31142	2.709448	1.327183
H	-1.4842	3.427286	1.347766
H	-3.25076	3.273482	1.34518
H	-2.2595	2.09603	2.232534
C	-2.31342	2.708412	-1.18464
H	-2.2631	2.094301	-2.0896
H	-3.25288	3.272282	-1.20135
H	-1.48619	3.426186	-1.20721
C	-9.14007	-3.43563	0.401992
H	-10.2019	-3.66233	0.413542
C	-8.19354	-4.39659	0.558506
C	9.140036	3.435601	0.401816
H	10.20184	3.662307	0.413288
C	8.193516	4.396548	0.55848
C	8.396431	5.85167	0.763727
H	7.962151	6.18506	1.711959
H	9.464016	6.082102	0.774941
H	7.926538	6.436645	-0.03361
C	-8.39645	-5.85172	0.763729
H	-7.92648	-6.43668	-0.03357
H	-7.96224	-6.1851	1.711994
H	-9.46403	-6.08216	0.77486
S	-6.55297	-3.76241	0.502303
S	6.552938	3.762369	0.502405
H	15.52486	-4.27749	-0.7279
H	13.50365	-5.67657	-0.85172
H	-15.5246	4.277651	-0.72824
H	-13.5033	5.676658	-0.85184

Table S2: Cartesian coordinates of **ATTD2.**

Atom	X-axis	Y-axis	Z-axis
C	1.552638	1.449256	0.125102
C	2.866492	1.025011	0.111581
C	3.180835	-0.34947	0.041245
C	2.182847	-1.32536	-0.01368
C	0.872378	-0.90209	-0.0016
C	0.555646	0.475533	0.065535

H	1.300415	2.50642	0.176608
H	2.435653	-2.38246	-0.06769
C	-0.88253	0.561947	0.052683
C	-1.45114	-0.68503	-0.02196
C	-2.8515	-0.66347	-0.06818
H	-3.48434	-1.54225	-0.14699
C	5.190608	0.814685	0.100357
C	6.582752	0.787248	0.080825
C	7.088443	-0.50197	-0.00383
H	7.220462	1.66555	0.112809
S	-2.06846	1.814818	0.082159
S	5.786094	-1.69141	-0.05438
C	4.617218	-0.43829	0.033108
C	-3.35909	0.620157	-0.0243
C	-0.38716	-1.75161	-0.05885
C	4.124111	1.878555	0.157507
C	-6.73468	2.270868	-0.23752
C	-5.30874	2.264617	-0.2291
C	-4.73273	1.02902	-0.04929
S	-6.00397	-0.15756	0.150069
C	10.99425	-0.89593	-0.04179
C	10.417	-2.16408	-0.27458
C	9.012586	-2.15028	-0.27454
S	9.709472	0.292155	0.187023
C	-7.27702	1.014355	-0.05399
C	8.454695	-0.89862	-0.05124
C	12.37649	-0.72531	-0.0303
C	13.22207	0.353345	0.159019
H	12.86967	-1.67452	-0.21567
C	14.66544	0.334395	0.111932
C	15.50487	-0.73142	-0.14872
C	15.39837	4.423071	0.973867
C	16.51845	3.624158	0.771348
C	16.40561	2.267081	0.480629
C	15.13471	1.710705	0.393958
C	14.01951	2.528672	0.599434
C	14.12472	3.872834	0.887035
H	17.30476	1.684323	0.330982
H	13.23058	4.469402	1.039214
C	12.79294	1.722053	0.457321
C	16.92033	-0.62606	-0.17391
N	18.0758	-0.59337	-0.20648
C	15.05728	-2.0503	-0.4238
N	14.72858	-3.13598	-0.65119
O	11.65357	2.134828	0.573483
C	4.207425	2.810281	-1.05122
H	3.38692	3.535997	-1.0351
H	5.152133	3.365684	-1.04016

H	4.150105	2.245056	-1.98717
C	4.205322	2.679305	1.456667
H	3.382801	3.400475	1.515948
H	4.149517	2.019342	2.328481
H	5.148757	3.235037	1.503628
C	-0.45519	-2.55825	-1.35505
H	0.362651	-3.28589	-1.4009
H	-1.40189	-3.10757	-1.41267
H	-0.38372	-1.90244	-2.22892
C	-0.48809	-2.67814	1.152485
H	-0.43809	-2.10902	2.08655
H	-1.43645	-3.22729	1.133528
H	0.328273	-3.40892	1.148727
C	-7.26395	3.578456	-0.50728
H	-8.32029	3.810087	-0.58732
C	-6.30993	4.517204	-0.67562
C	10.95307	-3.45641	-0.52752
H	12.01083	-3.69732	-0.57293
C	9.988775	-4.39427	-0.71507
C	10.16771	-5.83972	-0.99759
H	9.712899	-6.11931	-1.9535
H	11.2318	-6.08248	-1.03984
H	9.704067	-6.45865	-0.2225
C	-6.47932	5.963309	-0.9639
H	-6.03538	6.584622	-0.17847
H	-6.00216	6.24447	-1.90892
H	-7.54226	6.208137	-1.03184
S	-4.6657	3.867456	-0.52335
S	8.360935	-3.74036	-0.59348
H	17.50736	4.065453	0.841342
H	15.52311	5.477131	1.199073
C	-8.66943	0.601024	-0.01114
C	-9.07606	-0.65835	-0.469
C	-9.66179	1.452098	0.491666
C	-10.4008	-1.04462	-0.44523
H	-8.33998	-1.33872	-0.88949
C	-10.989	1.072936	0.521083
H	-9.38186	2.414837	0.909115
C	-11.3896	-0.18189	0.044401
H	-10.6828	-2.01982	-0.82944
H	-11.7311	1.748596	0.93464
N	-12.7346	-0.56051	0.059004
C	-13.1039	-1.92681	0.169976
C	-14.0071	-2.4877	-0.73508
C	-12.5879	-2.72562	1.182358
C	-14.3783	-3.81171	-0.62581
H	-14.4188	-1.86896	-1.52761
C	-12.9397	-4.06541	1.287824

H	-11.8917	-2.29576	1.897226
C	-13.843	-4.61572	0.38255
H	-15.0794	-4.25862	-1.32355
H	-12.5144	-4.66253	2.086282
C	-13.7637	0.409532	-0.0577
C	-14.8477	0.396244	0.810293
C	-13.7207	1.378365	-1.06384
C	-15.8738	1.326026	0.691774
H	-14.8931	-0.35803	1.59094
C	-14.7241	2.317425	-1.17614
H	-12.8852	1.390341	-1.75793
C	-15.8117	2.300135	-0.30035
H	-16.7074	1.286986	1.383842
H	-14.6989	3.075921	-1.95215
O	-16.7453	3.259498	-0.49803
O	-14.2599	-5.90276	0.397939
C	-17.8578	3.28498	0.367934
H	-17.5532	3.444296	1.40988
H	-18.4805	4.119672	0.04734
H	-18.4404	2.35746	0.303008
C	-13.7429	-6.7523	1.397871
H	-14.1936	-7.73093	1.235734
H	-12.6519	-6.84272	1.324175
H	-14.0059	-6.39841	2.402507

Table S3: Cartesian coordinates of **ATTD3.**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	0.456422	-0.98066	-0.40025
C	-0.83451	-0.49166	-0.39732
C	-1.08171	0.896051	-0.47598
C	-0.03741	1.82085	-0.55636
C	1.250637	1.333283	-0.55579
C	1.49885	-0.05775	-0.47947
H	0.6568	-2.04835	-0.34031
H	-0.23796	2.888845	-0.61426
C	2.929901	-0.21655	-0.49363
C	3.562057	0.998874	-0.57322
C	4.961027	0.902787	-0.60101
H	5.64195	1.745019	-0.67942
C	-3.14441	-0.16576	-0.34602
C	-4.53298	-0.06697	-0.30753
C	-4.97493	1.246603	-0.37837
H	-5.21195	-0.91205	-0.24392
S	4.046099	-1.52954	-0.43686
S	-3.61708	2.367209	-0.49381
C	-2.51156	1.056318	-0.44529
C	5.398549	-0.40552	-0.53697
C	2.552423	2.117118	-0.62526

C	-2.13142	-1.28117	-0.3127
C	8.673282	-2.25656	-0.64042
C	7.253882	-2.1548	-0.72218
C	6.746868	-0.89319	-0.517
S	8.074541	0.195722	-0.1798
C	-8.84684	1.861525	-0.15819
C	-8.22138	3.080615	-0.50445
C	-6.8239	2.984924	-0.60477
S	-7.61238	0.617047	0.051792
C	9.280993	-1.04889	-0.35761
C	-6.31821	1.71614	-0.35316
C	-10.2305	1.769864	-0.03652
C	-11.1131	0.752756	0.279955
H	-10.6908	2.726124	-0.26557
C	-12.5582	0.857602	0.368462
C	-13.3175	2.008494	0.368046
C	-14.0498	-2.60943	0.948043
C	-14.3052	-1.25542	0.608498
C	-13.0773	-0.5096	0.595521
C	-12.0054	-1.32519	0.827879
C	-10.7301	-0.61402	0.629118
C	-14.695	2.052852	0.702302
N	-15.8082	2.160656	0.995434
C	-12.7886	3.309299	0.145577
N	-12.4059	4.384492	-0.03973
O	-9.62013	-1.09529	0.732485
C	-2.29271	-2.2138	-1.51289
H	-1.50695	-2.97697	-1.51399
H	-3.26199	-2.72355	-1.47232
H	-2.23425	-1.65714	-2.45389
C	-2.21714	-2.07066	0.993253
H	-1.43251	-2.83398	1.034087
H	-2.1016	-1.41055	1.859026
H	-3.18662	-2.57586	1.070734
C	2.659454	2.899187	-1.93422
H	1.879133	3.666217	-1.99108
H	3.632704	3.398839	-2.00123
H	2.553551	2.234015	-2.79745
C	2.70027	3.056386	0.57111
H	2.623831	2.505638	1.514373
H	3.674166	3.558297	0.54272
H	1.920562	3.825874	0.556089
C	9.133809	-3.58473	-0.9368
H	10.17545	-3.88454	-0.96319
C	8.134303	-4.44894	-1.20765
C	-8.70345	4.388145	-0.78442
H	-9.74558	4.690578	-0.75742
C	-7.70609	5.257667	-1.09084

C	-7.82697	6.696379	-1.43239
H	-7.43419	6.903647	-2.43313
H	-8.87602	6.999151	-1.40595
H	-7.26996	7.322306	-0.72772
C	8.228797	-5.88958	-1.55274
H	7.692155	-6.51245	-0.82888
H	7.800077	-6.09637	-2.53926
H	9.275573	-6.20339	-1.56271
S	6.52981	-3.69792	-1.12889
S	-6.11263	4.516972	-1.05453
C	10.68955	-0.74357	-0.17393
C	11.22567	0.508864	-0.50006
C	11.56641	-1.7003	0.352995
C	12.56502	0.789359	-0.32209
H	10.58348	1.270108	-0.93568
C	12.90741	-1.42827	0.533497
H	11.17794	-2.66382	0.669512
C	13.43753	-0.17668	0.194874
H	12.95343	1.763642	-0.60197
H	13.55637	-2.18517	0.96255
N	14.79591	0.101642	0.368847
C	15.23495	1.417488	0.670522
C	16.28208	1.992484	-0.05242
C	14.65426	2.146667	1.700691
C	16.73336	3.25941	0.254098
H	16.74436	1.429632	-0.85844
C	15.0875	3.431736	2.002279
H	13.84522	1.705662	2.276194
C	16.13733	3.993969	1.281321
H	17.54818	3.715245	-0.29953
H	14.60811	3.973133	2.809213
C	15.76491	-0.93185	0.292275
C	16.73425	-1.06604	1.277463
C	15.78093	-1.81565	-0.79037
C	17.70829	-2.05411	1.196566
H	16.73231	-0.38159	2.121149
C	16.72934	-2.81374	-0.86681
H	15.03589	-1.71321	-1.57437
C	17.70488	-2.94124	0.124314
H	18.45474	-2.12833	1.979326
H	16.74925	-3.50622	-1.70243
O	18.5954	-3.94557	-0.04699
O	16.64678	5.228668	1.497894
C	19.59122	-4.11607	0.936764
H	19.15278	-4.32654	1.920267
H	20.19237	-4.96937	0.624332
H	20.23617	-3.23182	1.013912
C	16.08619	6.004239	2.533885

H	16.63653	6.944486	2.548065
H	15.02452	6.212925	2.351634
H	16.19242	5.511308	3.508391
C	-15.0581	-3.56241	1.028036
H	-14.8494	-4.59783	1.271525
C	-15.6267	-0.90941	0.289963
H	-15.9046	0.094024	0.001121
C	-16.6173	-1.85338	0.365843
C	-16.3427	-3.17668	0.737429
S	-12.3537	-2.96066	1.162442
N	-17.9977	-1.37259	0.172406
O	-18.1856	-0.58006	-0.72181
O	-18.8288	-1.76979	0.956658
N	-17.3603	-4.23615	0.669294
O	-18.1739	-4.15911	-0.22375
O	-17.2807	-5.13128	1.480468

Table S4: Cartesian coordinates of **ATTD4.**

Atom	X-axis	Y-axis	Z-axis
C	0.116887	-1.02876	0.153791
C	-1.17577	-0.54446	0.133566
C	-1.42754	0.839265	0.012643
C	-0.38601	1.764495	-0.08919
C	0.903994	1.281166	-0.07073
C	1.156841	-0.10548	0.049615
H	0.32002	-2.09382	0.244795
H	-0.58962	2.829453	-0.18239
C	2.588837	-0.26012	0.032192
C	3.216376	0.953405	-0.09585
C	4.614758	0.859893	-0.14517
H	5.290491	1.701808	-0.26231
C	-3.48787	-0.22748	0.137852
C	-4.87865	-0.13594	0.138381
C	-5.32567	1.171095	0.017603
H	-5.55402	-0.98283	0.214651
S	3.709939	-1.56758	0.111504
S	-3.97121	2.295771	-0.0956
C	-2.85914	0.993537	0.01782
C	5.058295	-0.44457	-0.04898
C	2.202719	2.066688	-0.17179
C	-2.4708	-1.33647	0.224537
C	8.334814	-2.2921	-0.18511
C	6.911865	-2.20153	-0.18304
C	6.408225	-0.92805	-0.05774
S	7.746694	0.189702	0.096107
C	-9.21007	1.753175	0.035527
C	-8.57865	2.989763	-0.20807
C	-7.17498	2.907703	-0.2341

S	-7.98131	0.506181	0.245534
C	8.949457	-1.06274	-0.05125
C	-6.67347	1.632938	-0.01629
C	-10.6025	1.645484	0.072482
C	-11.4891	0.608541	0.267414
H	-11.0578	2.611352	-0.12443
C	-12.9408	0.695178	0.270902
C	-13.7103	1.837431	0.341467
C	-14.4376	-2.80921	0.371091
C	-14.6755	-1.42847	0.158502
C	-13.4541	-0.68664	0.323638
C	-12.3938	-1.51688	0.561572
C	-11.1192	-0.78663	0.526584
C	-15.1022	1.842492	0.616385
N	-16.2267	1.918475	0.874209
C	-13.1786	3.154557	0.277579
N	-12.7904	4.242131	0.218176
O	-10.0107	-1.26192	0.669007
C	-2.60968	-2.31034	-0.94492
H	-1.82213	-3.07083	-0.90709
H	-3.57816	-2.82151	-0.90269
H	-2.53735	-1.78596	-1.90337
C	-2.5741	-2.08067	1.555684
H	-1.78812	-2.83968	1.635186
H	-2.47365	-1.38997	2.399266
H	-3.54346	-2.58573	1.636267
C	2.297983	2.811389	-1.50318
H	1.517107	3.576573	-1.57567
H	3.270412	3.309149	-1.59285
H	2.185095	2.121656	-2.34605
C	2.356098	3.039898	0.996335
H	2.287504	2.515776	1.955254
H	3.328317	3.543507	0.947123
H	1.573817	3.806315	0.964687
C	8.786491	-3.63994	-0.39283
H	9.827265	-3.93696	-0.45867
C	7.779216	-4.52766	-0.52073
C	-9.05474	4.31091	-0.43843
H	-10.0994	4.605599	-0.44976
C	-8.0502	5.201604	-0.63668
C	-8.16259	6.657213	-0.90161
H	-7.72316	6.922254	-1.86885
H	-9.21339	6.955194	-0.90919
H	-7.64402	7.244081	-0.13651
C	7.863541	-5.99316	-0.74143
H	7.376018	-6.55017	0.066066
H	7.378402	-6.28833	-1.67809
H	8.910224	-6.30436	-0.786

S	6.176785	-3.77632	-0.40596
S	-6.45318	4.46815	-0.55331
C	10.3646	-0.7344	-0.01212
C	10.85532	0.475228	-0.51883
C	11.29619	-1.62473	0.53708
C	12.20219	0.775707	-0.49874
H	10.16765	1.183157	-0.9744
C	12.64469	-1.33259	0.561975
H	10.95133	-2.54783	0.993396
C	13.12953	-0.12777	0.036379
H	12.54984	1.713263	-0.92088
H	13.33826	-2.0365	1.010847
N	14.49668	0.156651	0.046519
C	14.97122	1.494113	0.056845
C	15.94413	1.900825	-0.85887
C	14.50113	2.415766	0.983929
C	16.42961	3.191825	-0.84193
H	16.32084	1.187505	-1.58646
C	14.96765	3.724251	0.993697
H	13.75241	2.10913	1.70894
C	15.94148	4.119098	0.080052
H	17.18643	3.51663	-1.54906
H	14.57458	4.418354	1.727397
C	15.45354	-0.89228	-0.00334
C	16.49382	-0.93996	0.914703
C	15.38432	-1.87423	-0.99454
C	17.45633	-1.94095	0.856583
H	16.55685	-0.1765	1.685245
C	16.32345	-2.88245	-1.04847
H	14.58058	-1.83933	-1.72471
C	17.37044	-2.92425	-0.12481
H	18.25852	-1.94908	1.585854
H	16.27971	-3.65133	-1.81333
O	18.2436	-3.94723	-0.26844
O	16.47093	5.362361	0.008478
C	19.30873	-4.03976	0.651153
H	18.94328	-4.16344	1.678196
H	19.88475	-4.92068	0.369524
H	19.95896	-3.15721	0.605566
C	16.00149	6.333428	0.917177
H	16.54123	7.252959	0.69266
H	14.92528	6.509918	0.796624
H	16.20248	6.043888	1.956217
C	-15.4423	-3.76022	0.263927
H	-15.2444	-4.81169	0.438655
C	-15.9618	-1.04977	-0.24273
H	-16.2013	-0.02239	-0.47478
C	-16.9597	-1.99196	-0.35866

C	-16.7087	-3.34833	-0.0934
S	-12.7561	-3.17993	0.698036
Cl	-17.9638	-4.53564	-0.23777
Cl	-18.5399	-1.46414	-0.84749

Table S5: Cartesian coordinates of **ATTD5.**

Atom	X-axis	Y-axis	Z-axis
C	0.991879	-1.00829	-0.22681
C	-0.29273	-0.50253	-0.21442
C	-0.52014	0.890271	-0.24209
C	0.536392	1.803169	-0.28631
C	1.817826	1.29877	-0.29788
C	2.047261	-0.09718	-0.26618
H	1.178054	-2.08	-0.2037
H	0.349902	2.875079	-0.30736
C	3.476233	-0.27388	-0.27754
C	4.124847	0.934783	-0.31587
C	5.522254	0.822288	-0.31741
H	6.211649	1.660854	-0.34487
C	-2.59943	-0.14412	-0.16135
C	-3.98693	-0.02373	-0.11423
C	-4.40726	1.298964	-0.12256
H	-4.67889	-0.85972	-0.07378
S	4.575352	-1.60137	-0.23989
S	-3.02977	2.399749	-0.19353
C	-1.94713	1.070155	-0.20742
C	5.944784	-0.49284	-0.27649
C	3.130017	2.067221	-0.33569
C	-1.60236	-1.27512	-0.16821
C	9.191421	-2.39667	-0.19835
C	7.770258	-2.28372	-0.22142
C	7.286934	-0.99621	-0.25098
S	8.644229	0.109973	-0.23301
C	-8.2707	1.986501	0.065745
C	-7.60138	3.226247	-0.0134
C	-6.2034	3.104384	-0.08831
S	-7.0819	0.682755	0.043406
C	9.825747	-1.17104	-0.20614
C	-5.74115	1.795349	-0.07093
C	-9.65986	1.921442	0.16849
C	-10.581	0.898934	0.276925
H	-10.083	2.920489	0.139508
C	-12.0187	1.041295	0.429568
C	-12.7192	2.188993	0.735693
C	-13.677	-2.38351	0.19302
C	-13.8649	-0.98366	0.20828
C	-12.598	-0.31481	0.336288
C	-11.5647	-1.20967	0.335255

C	-10.2604	-0.53009	0.283814
C	-14.081	2.208892	1.132756
N	-15.1743	2.294105	1.499032
C	-12.1306	3.481196	0.810673
N	-11.6971	4.551419	0.87072
O	-9.17125	-1.06572	0.240656
C	-1.77011	-2.15493	-1.40697
H	-0.99519	-2.92863	-1.4367
H	-2.7469	-2.65164	-1.3926
H	-1.69893	-1.56009	-2.32343
C	-1.70731	-2.11642	1.103324
H	-0.93203	-2.89016	1.11792
H	-1.59027	-1.49411	1.996453
H	-2.68323	-2.61258	1.153256
C	3.252902	2.892847	-1.61602
H	2.481727	3.670397	-1.64977
H	4.232304	3.382868	-1.66084
H	3.143634	2.259581	-2.50248
C	3.28493	2.962371	0.893407
H	3.198888	2.379563	1.816363
H	4.264782	3.453385	0.88591
H	2.514495	3.741237	0.903638
C	9.623331	-3.76615	-0.22276
H	10.66034	-4.08302	-0.23771
C	8.602981	-4.64763	-0.24395
C	-8.03471	4.581073	-0.01751
H	-9.06794	4.908002	0.043652
C	-7.00259	5.459435	-0.0945
C	-7.06894	6.941435	-0.11902
H	-6.62592	7.346315	-1.03484
H	-8.10971	7.268666	-0.06705
H	-6.52794	7.379609	0.726047
C	8.664891	-6.13036	-0.27369
H	8.167846	-6.57162	0.59711
H	8.176552	-6.53604	-1.16639
H	9.706889	-6.45979	-0.27458
S	7.011809	-3.86307	-0.24306
S	-5.4324	4.671161	-0.16704
C	11.24466	-0.86025	-0.16656
C	11.7711	0.267029	-0.80954
C	12.14008	-1.67663	0.535632
C	13.11798	0.562361	-0.76248
H	11.11203	0.910214	-1.38722
C	13.48907	-1.38753	0.590333
H	11.76253	-2.53153	1.08916
C	14.00848	-0.26019	-0.05927
H	13.49642	1.434474	-1.28642
H	14.15198	-2.02815	1.16333

N	15.3705	0.042408	-0.00524
C	15.8189	1.388412	-0.07862
C	16.82517	1.743882	-0.97871
C	15.28961	2.365808	0.75425
C	17.28738	3.04225	-1.03745
H	17.24574	0.984644	-1.63226
C	15.73362	3.680466	0.687891
H	14.51254	2.09769	1.464661
C	16.74243	4.024526	-0.20804
H	18.07042	3.329782	-1.73199
H	15.29684	4.420366	1.348468
C	16.34109	-0.97413	0.192342
C	17.31702	-0.83467	1.170282
C	16.35491	-2.11632	-0.61232
C	18.29596	-1.80394	1.350249
H	17.31662	0.052069	1.798091
C	17.31047	-3.09362	-0.42666
H	15.60362	-2.23259	-1.38836
C	18.29317	-2.94563	0.554729
H	19.04605	-1.65998	2.119027
H	17.33004	-3.98467	-1.04627
O	19.19206	-3.95253	0.652622
O	17.25529	5.268867	-0.34602
C	20.19874	-3.84283	1.634296
H	19.7721	-3.79226	2.643846
H	20.81142	-4.73987	1.55073
H	20.82919	-2.96066	1.467134
C	16.74311	6.288717	0.48273
H	17.28331	7.198571	0.222963
H	15.67083	6.445816	0.311238
H	16.90664	6.064146	1.54415
C	-14.7404	-3.26901	0.080168
H	-14.5636	-4.33783	0.086841
C	-15.1715	-0.51491	0.020746
H	-15.3652	0.545691	-0.03279
C	-16.2355	-1.38396	-0.09718
C	-16.0236	-2.78235	-0.05895
S	-11.9967	-2.85983	0.270487
C	-17.1342	-3.79961	-0.1206
C	-17.5917	-0.76241	-0.31714
F	-16.6597	-5.02232	-0.37382
F	-18.0248	-3.52842	-1.07439
F	-17.793	-3.87881	1.038354
F	-17.9804	-0.86199	-1.59194
F	-18.5347	-1.32978	0.437048
F	-17.5901	0.537026	-0.01852

Table S6: Cartesian coordinates of **ATTD6.**

Atom	X-axis	Y-axis	Z-axis
C	-1.38674	-0.84903	0.381327
C	-0.10479	-0.33691	0.369936
C	0.116917	1.055944	0.43008
C	-0.94361	1.962778	0.500365
C	-2.22265	1.452109	0.508582
C	-2.44552	0.055928	0.450369
H	-1.56811	-1.92083	0.335652
H	-0.76197	3.034834	0.544133
C	-3.87329	-0.12899	0.469608
C	-4.52775	1.075215	0.535278
C	-5.92478	0.953289	0.566125
H	-6.62094	1.783867	0.634325
C	2.199144	0.031759	0.311222
C	3.585821	0.157149	0.270515
C	4.002218	1.480121	0.323022
H	4.281266	-0.6752	0.218393
S	-4.96438	-1.4632	0.431103
S	2.622494	2.575164	0.423976
C	1.543246	1.242546	0.394802
C	-6.33798	-0.36389	0.518391
C	-3.53871	2.21247	0.570622
C	1.206927	-1.10282	0.294121
C	-9.5751	-2.27947	0.634367
C	-8.15774	-2.15008	0.710352
C	-7.67667	-0.87802	0.505478
S	-9.02778	0.185113	0.176769
C	7.862493	2.168138	0.112891
C	7.211632	3.379799	0.435421
C	5.815551	3.259055	0.527296
S	6.654271	0.897403	-0.08846
C	-10.2079	-1.08405	0.356452
C	5.336144	1.976363	0.294182
C	9.249179	2.099309	0.012645
C	10.15411	1.095333	-0.28007
H	9.690242	3.065236	0.23979
C	11.59773	1.227134	-0.34029
C	12.34173	2.388096	-0.33953
C	13.17624	-2.19963	-0.89186
C	13.38546	-0.84885	-0.53104
C	12.14402	-0.12963	-0.5513
C	11.09693	-0.96495	-0.82013
C	9.803247	-0.27844	-0.64126
C	13.72095	2.441875	-0.66818
N	14.83402	2.548691	-0.96241
C	11.7921	3.682801	-0.13425
N	11.38898	4.752555	0.038618
O	8.704131	-0.77838	-0.76608

C	1.38717	-2.0156	1.50691
H	0.615688	-2.79309	1.520428
H	2.365681	-2.50782	1.471783
H	1.320021	-1.44689	2.440121
C	1.305944	-1.90835	-1.00101
H	0.535023	-2.68599	-1.03076
H	1.17791	-1.26226	-1.87554
H	2.284264	-2.39708	-1.07255
C	-3.65767	3.010012	1.869125
H	-2.89118	3.791622	1.914257
H	-4.63965	3.492914	1.931244
H	-3.5383	2.358586	2.741008
C	-3.70632	3.13258	-0.63809
H	-3.62224	2.5704	-1.57394
H	-4.68911	3.617092	-0.61407
H	-2.94069	3.916209	-0.63589
C	-10.0091	-3.61665	0.930377
H	-11.0449	-3.93586	0.961046
C	-8.9923	-4.46212	1.195132
C	7.667311	4.700336	0.69856
H	8.704072	5.021139	0.674526
C	6.65168	5.555757	0.983374
C	6.743081	7.001945	1.302074
H	6.335912	7.218771	2.294979
H	7.786735	7.323263	1.281459
H	6.182701	7.605963	0.58113
C	-9.05747	-5.90461	1.539354
H	-8.51317	-6.51667	0.812037
H	-8.61944	-6.1039	2.523328
H	-10.098	-6.23833	1.554953
S	-7.40276	-3.68039	1.109868
S	5.072411	4.7849	0.946372
C	-11.6239	-0.80914	0.180378
C	-12.1888	0.424878	0.526415
C	-12.479	-1.77943	-0.35742
C	-13.5357	0.674534	0.358617
H	-11.5633	1.195308	0.970099
C	-13.8271	-1.53803	-0.52851
H	-12.0682	-2.72855	-0.68906
C	-14.3867	-0.3055	-0.16842
H	-13.9467	1.634596	0.654913
H	-14.4589	-2.30467	-0.96579
N	-15.7525	-0.05928	-0.33103
C	-16.2281	1.24908	-0.6102
C	-17.2877	1.782532	0.126537
C	-15.675	2.008829	-1.63322
C	-17.7798	3.038468	-0.16136
H	-17.7275	1.195203	0.927605

C	-16.1498	3.283574	-1.9163
H	-14.856	1.599858	-2.2182
C	-17.213	3.80306	-1.18302
H	-18.6052	3.462036	0.402176
H	-15.6936	3.851415	-2.71875
C	-16.6948	-1.11852	-0.27321
C	-17.6636	-1.25595	-1.25844
C	-16.6869	-2.02414	0.791458
C	-18.615	-2.26708	-1.19445
H	-17.6801	-0.5547	-2.08807
C	-17.6122	-3.04482	0.850534
H	-15.9423	-1.92017	1.575741
C	-18.5885	-3.1744	-0.13955
H	-19.3619	-2.34261	-1.97665
H	-17.6138	-3.75387	1.672397
O	-19.4572	-4.20019	0.016164
O	-17.7625	5.02332	-1.38262
C	-20.4564	-4.3707	-0.96412
H	-20.0212	-4.55674	-1.95397
H	-21.0407	-5.23957	-0.66277
H	-21.1171	-3.49667	-1.0215
C	-17.2338	5.825467	-2.41493
H	-17.8099	6.750206	-2.41374
H	-16.1765	6.061049	-2.24041
H	-17.3359	5.340045	-3.39365
C	14.21594	-3.12003	-0.95105
H	14.02948	-4.14968	-1.23655
C	14.68289	-0.48354	-0.15213
H	14.8935	0.518243	0.194439
C	15.71632	-1.39424	-0.19271
C	15.49566	-2.72447	-0.62344
S	11.49628	-2.58938	-1.16159
S	16.65396	-4.09638	-0.52644
O	16.95393	-4.32994	0.867008
O	16.132	-5.15308	-1.34908
O	17.96258	-3.58557	-1.27876
H	18.52165	-3.07504	-0.66175
S	17.30526	-0.62052	0.090205
O	17.95686	-0.40522	-1.17183
O	17.12832	0.441729	1.042612
O	18.18782	-1.79336	0.76615
H	17.93078	-1.99047	1.681208

Table S7: Cartesian coordinates of **ATTD7.**

Atom	**X-axis**	**Y-axis**	**Z-axis**
C	0.101856	-1.03693	-0.04097
C	1.3965	-0.55828	-0.03027
C	1.654513	0.827115	0.055888

C	0.616698	1.759833	0.130953
C	-0.67517	1.28237	0.12077
C	-0.93382	-0.10632	0.036344
H	-0.10632	-2.10289	-0.10522
H	0.825252	2.825842	0.196639
C	-2.36573	-0.25457	0.051701
C	-2.98911	0.964616	0.143469
C	-4.38799	0.877752	0.186392
H	-5.0613	1.724979	0.2759
C	3.709296	-0.25338	-0.04091
C	5.0989	-0.16897	-0.04366
C	5.553118	1.139306	0.045565
H	5.769748	-1.02121	-0.09652
S	-3.49131	-1.55961	0.001072
S	4.204235	2.273523	0.131077
C	3.086204	0.974548	0.049044
C	-4.83576	-0.42753	0.122398
C	-1.97119	2.075564	0.194029
C	2.687121	-1.35912	-0.09877
C	-8.11771	-2.26285	0.275498
C	-6.6949	-2.17475	0.290478
C	-6.18699	-0.90654	0.131599
S	-7.52131	0.208261	-0.07531
C	9.440298	1.6904	-0.00518
C	8.818997	2.932871	0.251916
C	7.416515	2.86175	0.287211
S	8.197353	0.455128	-0.21785
C	-8.72792	-1.03729	0.094301
C	6.902534	1.590689	0.066864
C	10.82697	1.569483	-0.04767
C	11.70371	0.521324	-0.25959
H	11.29455	2.527623	0.158127
C	13.15367	0.592579	-0.26892
C	13.94031	1.724078	-0.30989
C	14.59957	-2.93259	-0.49216
C	14.86189	-1.56092	-0.23359
C	13.65341	-0.79528	-0.36965
C	12.58199	-1.60385	-0.62476
C	11.31371	-0.85695	-0.55446
C	15.32933	1.708931	-0.59629
N	16.45326	1.761818	-0.86186
C	13.4305	3.046717	-0.20145
N	13.05818	4.137129	-0.10565
O	10.20173	-1.32137	-0.70273
C	2.820205	-2.30102	1.097528
H	2.028052	-3.0574	1.080556
H	3.785514	-2.81909	1.069589
H	2.750999	-1.75	2.041118

C	2.787523	-2.1407	-1.40847
H	1.996241	-2.89593	-1.46784
H	2.693409	-1.47359	-2.27149
H	3.753286	-2.65482	-1.47276
C	-2.06967	2.85809	1.503226
H	-1.28432	3.62008	1.558368
H	-3.03939	3.364237	1.572679
H	-1.96613	2.192206	2.366187
C	-2.11488	3.016155	-1.00193
H	-2.0445	2.464941	-1.94539
H	-3.08505	3.525126	-0.97138
H	-1.32931	3.779715	-0.98837
C	-8.57545	-3.60223	0.521216
H	-9.61768	-3.89532	0.581592
C	-7.5721	-4.48682	0.693687
C	9.307617	4.24638	0.490712
H	10.3547	4.53259	0.498413
C	8.310693	5.143816	0.703959
C	8.437229	6.596074	0.980053
H	8.005416	6.856823	1.951825
H	9.490539	6.884893	0.98407
H	7.919375	7.193341	0.222616
C	-7.66238	-5.94369	0.963539
H	-7.16388	-6.52898	0.183244
H	-7.19171	-6.20674	1.917011
H	-8.71016	-6.25175	1.003582
S	-5.96657	-3.74246	0.576278
S	6.709037	4.423668	0.625672
C	-10.1421	-0.7107	0.023614
C	-10.6426	0.511072	0.489949
C	-11.0634	-1.61699	-0.51676
C	-11.9896	0.807616	0.440845
H	-9.96307	1.232126	0.937157
C	-12.4116	-1.32884	-0.57115
H	-10.7094	-2.55105	-0.94282
C	-12.9071	-0.11184	-0.08427
H	-12.3456	1.755034	0.832825
H	-13.0965	-2.04582	-1.01251
N	-14.2742	0.168629	-0.12238
C	-14.7516	1.504843	-0.15947
C	-15.7306	1.925418	0.743235
C	-14.278	2.410841	-1.09989
C	-16.2185	3.214941	0.700825
H	-16.1103	1.224189	1.48097
C	-14.7473	3.717876	-1.13574
H	-13.5242	2.092704	-1.81464
C	-15.7271	4.126905	-0.23471
H	-16.98	3.550685	1.397744

H	-14.3511	4.399086	-1.87979
C	-15.2305	-0.88072	-0.06872
C	-16.2565	-0.94486	-1.0016
C	-15.1766	-1.84495	0.94077
C	-17.2195	-1.94525	-0.94109
H	-16.3079	-0.19484	-1.78609
C	-16.1159	-2.85292	0.997333
H	-14.385	-1.79641	1.683342
C	-17.1481	-2.91169	0.058139
H	-18.0104	-1.96642	-1.68228
H	-16.0838	-3.6083	1.776098
O	-18.0227	-3.9328	0.205557
O	-16.2597	5.369831	-0.18808
C	-19.0732	-4.04191	-0.72905
H	-18.6914	-4.18191	-1.74799
H	-19.6526	-4.91881	-0.44202
H	-19.7248	-3.15945	-0.7081
C	-15.7885	6.326114	-1.1116
H	-16.3321	7.247773	-0.90602
H	-14.7135	6.508221	-0.98883
H	-15.9836	6.017749	-2.14631
C	15.58546	-3.90715	-0.43183
H	15.36144	-4.94469	-0.65206
C	16.15484	-1.21678	0.181148
H	16.40633	-0.20103	0.45131
C	17.13982	-2.18314	0.263629
C	16.86476	-3.53455	-0.06207
S	12.91545	-3.2656	-0.8171
C	18.44881	-1.81133	0.691865
N	19.5083	-1.51685	1.039679
C	17.89181	-4.51916	0.014025
N	18.72035	-5.31956	0.073742

Table S8: Cartesian coordinates of **ATTD8.**

Atom	X-axis	Y-axis	Z-axis
C	-0.93259	-0.95893	0.477394
C	0.357253	-0.46669	0.471895
C	0.599775	0.923328	0.508118
C	-0.44732	1.846784	0.55115
C	-1.73452	1.355727	0.554192
C	-1.97832	-0.0371	0.5172
H	-1.12975	-2.02856	0.448577
H	-0.24995	2.916622	0.577847
C	-3.40964	-0.199	0.520209
C	-4.04556	1.016144	0.557794
C	-5.44475	0.917158	0.567892
H	-6.12786	1.760247	0.610758

C	2.667367	-0.13389	0.428671
C	4.057617	-0.03087	0.393873
C	4.493401	1.285133	0.419098
H	4.740331	-0.87476	0.361917
S	-4.52188	-1.51569	0.483192
S	3.13083	2.403306	0.487085
C	2.029977	1.087049	0.481715
C	-5.87897	-0.39334	0.531771
C	-3.03881	2.137929	0.587709
C	1.658052	-1.25358	0.425187
C	-9.14709	-2.25825	0.594469
C	-7.72893	-2.15137	0.690005
C	-7.22571	-0.8854	0.502465
S	-8.5565	0.202048	0.169509
C	8.361314	1.924455	0.174252
C	7.726727	3.150211	0.460823
C	6.328712	3.046105	0.569735
S	7.142062	0.658439	0.035582
C	-9.75782	-1.05064	0.321372
C	5.835483	1.764165	0.378037
C	9.747762	1.84822	0.020711
C	10.63889	0.834927	-0.25831
H	10.19434	2.824795	0.179342
C	12.07806	0.964369	-0.42388
C	12.79937	2.127015	-0.59418
C	13.66282	-2.49258	-0.68306
C	13.87869	-1.10345	-0.50804
C	12.62296	-0.40264	-0.52531
C	11.56891	-1.26666	-0.63257
C	10.28395	-0.57346	-0.46185
C	14.15115	2.173511	-1.02445
N	15.23441	2.292301	-1.41055
C	12.23851	3.429136	-0.48583
N	11.82796	4.506381	-0.39594
O	9.180878	-1.08153	-0.47364
C	1.811989	-2.14333	1.658575
H	1.028233	-2.90834	1.680641
H	2.783049	-2.65118	1.643913
H	1.744634	-1.55382	2.578764
C	1.757897	-2.08791	-0.8514
H	0.974813	-2.85361	-0.87332
H	1.650023	-1.45865	-1.74083
H	2.728919	-2.5936	-0.90169
C	-3.16041	2.958521	1.871478
H	-2.38071	3.727117	1.91386
H	-4.13444	3.459477	1.912917
H	-3.0638	2.319562	2.755339
C	-3.17685	3.040871	-0.63757

H	-3.0911	2.461994	-1.56302
H	-4.15162	3.541972	-0.6334
H	-2.39826	3.811672	-0.6389
C	-9.60568	-3.59151	0.869363
H	-10.6468	-3.89437	0.881176
C	-8.60554	-4.4553	1.138673
C	8.195698	4.477212	0.669975
H	9.234712	4.787732	0.622453
C	7.191435	5.351028	0.933568
C	7.298029	6.806598	1.201127
H	6.90171	7.061278	2.189533
H	8.344192	7.117889	1.160308
H	6.736448	7.390624	0.464709
C	-8.69766	-5.90034	1.465644
H	-8.15363	-6.5128	0.738439
H	-8.2756	-6.11754	2.45281
H	-9.74345	-6.21761	1.46411
S	-7.00302	-3.69747	1.083629
S	5.603272	4.593901	0.940065
C	-11.1674	-0.75415	0.12894
C	-11.7258	0.475817	0.497884
C	-12.0224	-1.70167	-0.44814
C	-13.0677	0.743003	0.315394
H	-11.1001	1.227547	0.972366
C	-13.3644	-1.44156	-0.63679
H	-11.6147	-2.64683	-0.79484
C	-13.9185	-0.21344	-0.25297
H	-13.4737	1.698254	0.632666
H	-13.9965	-2.1899	-1.10453
N	-15.2809	0.043647	-0.43132
C	-15.7598	1.362716	-0.64047
C	-16.8577	1.833203	0.083871
C	-15.173	2.200457	-1.58093
C	-17.3525	3.10208	-0.13437
H	-17.3259	1.185079	0.81924
C	-15.6501	3.488462	-1.79053
H	-14.3248	1.843968	-2.15839
C	-16.7505	3.944746	-1.07038
H	-18.2073	3.474975	0.421046
H	-15.1661	4.117686	-2.52856
C	-16.2261	-1.01478	-0.38617
C	-17.1841	-1.1477	-1.38234
C	-16.2316	-1.92171	0.676959
C	-18.1389	-2.15609	-1.33011
H	-17.1895	-0.44456	-2.21054
C	-17.1603	-2.93992	0.724881
H	-15.4944	-1.82072	1.468525
C	-18.1262	-3.06484	-0.27588

H	-18.8777	-2.22888	-2.1203
H	-17.1727	-3.65058	1.545229
O	-18.999	-4.08834	-0.13091
O	-17.3041	5.17247	-1.20565
C	-19.9895	-4.25437	-1.12082
H	-19.5457	-4.44096	-2.10668
H	-20.5796	-5.12151	-0.82583
H	-20.6466	-3.37794	-1.1834
C	-16.7397	6.049623	-2.15452
H	-17.3258	6.967283	-2.11466
H	-15.6939	6.281468	-1.9171
H	-16.793	5.633427	-3.16834
C	14.70876	-3.40782	-0.70364
H	14.52417	-4.46606	-0.85971
C	15.18981	-0.68277	-0.2523
H	15.40648	0.348566	-0.01525
C	16.23476	-1.58691	-0.26214
C	15.99742	-2.95172	-0.52556
S	11.96962	-2.91837	-0.80369
C	17.59632	-1.15002	0.148885
O	18.43711	-1.89013	0.594937
O	17.76488	0.161499	0.000732
C	17.09847	-3.9554	-0.61688
O	17.14508	-4.96238	0.037245
O	17.97131	-3.62274	-1.56482
C	19.02076	0.683063	0.435342
H	19.15806	0.508182	1.504905
H	19.83972	0.21257	-0.11292
H	18.98819	1.75019	0.226625
C	19.14914	-4.42713	-1.61937
H	19.71335	-4.30848	-0.69019
H	18.89583	-5.47978	-1.76044
H	19.72871	-4.05804	-2.46294

Table S9: Calculated energies (E) and energy gap (ΔE) of HOMO-1, LUMO+1, HOMO-2 and LUMO+2 for **ATTR1** and **ATTD2-ATTD8** at **M06/6-31G (d,p)**.

Compounds	**HOMO-1**	**LUMO+1**	ΔE	**HOMO-2**	**LUMO+2**	ΔE
ATTR1	-6.071	-3.217	2.854	-6.713	-2.604	4.109
ATTD2	-5.588	-2.517	3.071	-5.95	-2.034	3.916
ATTD3	-5.629	-3.27	2.359	-6.009	-2.836	3.173
ATTD4	-5.586	-2.957	2.629	-5.948	-2.033	3.915
ATTD5	-5.604	-3.047	2.557	-5.974	-2.074	3.9
ATTD6	-5.624	-3.169	2.455	-6.004	-2.204	3.8
ATTD7	-5.631	-3.177	2.454	-6.003	-2.281	3.722
ATTD8	-5.575	-2.959	2.616	-5.943	-2.040	3.903

E=energy, ΔE (eV) =E_{LUMO}-E_{HOMO}; HOMO=highest occupied molecular orbital; LUMO=lowest unoccupied molecular orbital, MO=molecular orbital, Units in eV

Table S10: Wavelength, excitation energy and oscillator strength of **ATTR1** in chloroform solvent at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	751.510	1.650	3.297	H→L (93%), H-1→L+1 (5%)
2	620.666	1.998	0.003	H→L+1 (90%), H-1→L (8%)
3	559.394	2.216	0.002	H-1→L (88%), H-2→L+1 (3%), H→L+1 (8%)
4	507.176	2.445	0.053	H-1→L+1 (54%), H→L+2 (32%), H-2→L (3%), H-1→L+3 (6%), H→L (2%)
5	498.429	2.488	0.272	H-1→L+1 (35%), H→L+2 (50%), H-1→L+3 (8%), H→L (3%)
6	491.708	2.522	0.001	H-1→L+2 (16%), H→L+3 (79%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S11: Wavelength, excitation energy and oscillator strength of **ATTD2** in chloroform solvent at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	818.864	1.514	1.578	H→L (92%), H-1→L (6%)
2	637.385	1.945	0.871	H-2→L (12%), H-1→L (78%), H→L (7%)
3	551.580	2.248	0.249	H-1→L+1 (10%), H→L+1 (79%), H-2→L+1 (3%), H→L+2 (5%)
4	531.984	2.331	0.115	H-2→L (82%), H-1→L (13%), H-3→L (4%)
5	499.775	2.481	0.700	H→L+2 (85%), H-1→L+1 (3%), H→L+1 (3%), H→L+3 (3%)
6	472.789	2.622	0.043	H-2→L+1 (19%), H-1→L+1 (59%), H→L+1 (17%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S12: Wavelength, excitation energy and oscillator strength of **ATTD3** in chloroform solvent at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	846.944	1.464	1.399	H→L (92%), H-1→L (5%)
2	781.052	1.587	0.035	H→L+1 (88%), H-2→L+1 (3%), H-1→L+1 (8%)
3	655.446	1.892	0.797	H-2→L (12%), H-1→L (65%), H-2→L+1 (3%), H-1→L+1 (7%), H→L (6%), H→L+1 (2%)
4	636.306	1.949	0.350	H-2→L+1 (16%), H-1→L+1 (49%), H→L+1 (10%), H-1→L (8%), H-1→L+2 (2%), H→L+2 (9%)
5	600.030	2.066	0.044	H→L+2 (84%), H-1→L (5%), H-1→L+1 (7%)
6	542.719	2.285	0.190	H-2→L (77%), H-1→L (14%), H-3→L (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S13: Wavelength, excitation energy and oscillator strength of **ATTD4** in chloroform solvent at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions

1	799.434	1.551	1.465	H→L (88%), H-1→L (8%)
2	690.835	1.795	0.324	H-1→L+1 (13%), H→L+1 (78%), H-2→L+1 (4%)
3	632.766	1.959	0.635	H-2→L (14%), H-1→L (68%), H→L (11%), H→L+1 (3%)
4	570.514	2.173	0.296	H-2→L+1 (16%), H-1→L+1 (59%), H→L+1 (17%), H-1→L (3%)
5	520.133	2.384	0.125	H-2→L (76%), H-1→L (16%), H-3→L (4%)
6	503.612	2.462	0.832	H→L+2 (90%), H→L+3 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S14: Wavelength, excitation energy and oscillator strength of **ATTD5** in chloroform solvent at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	816.169	1.519	1.474	H→L (90%), H-1→L (6%)
2	713.825	1.737	0.262	H-1→L+1 (11%), H→L+1 (82%), H-2→L+1 (4%)
3	638.337	1.942	0.640	H-2→L (15%), H-1→L (70%), H→L (9%), H→L+1 (2%)
4	584.170	2.122	0.291	H-2→L+1 (18%), H-1→L+1 (60%), H→L+1 (14%), H-1→L (4%)
5	528.627	2.345	0.159	H-2→L (75%), H-1→L (17%), H-3→L (4%)
6	506.079	2.450	0.812	H→L+2 (87%), H→L+3 (6%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S15: Wavelength, excitation energy and oscillator strength of **ATTD6** in chloroform solvent at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	E(*eV*)	f_{os}	MO contributions
1	835.698	1.484	1.368	H→L (90%), H-1→L (6%)
2	749.104	1.655	0.216	H→L+1 (85%), H-2→L+1 (3%), H-1→L+1 (9%)
3	651.725	1.902	0.658	H-2→L (16%), H-1→L (69%), H→L (8%)
4	609.349	2.035	0.387	H-2→L+1 (19%), H-1→L+1 (61%), H→L+1 (12%), H-1→L (4%)
5	539.296	2.299	0.181	H-2→L (75%), H-1→L (18%), H-3→L (4%)
6	509.887	2.432	0.819	H→L+2 (53%), H→L+3 (34%), H-1→L+1 (4%), H→L+4 (2%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S16: Wavelength, excitation energy and oscillator strength of **ATTD7** in chloroform solvent at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	836.093	1.483	1.431	H→L (90%), H-1→L (6%)
2	754.850	1.643	0.201	H→L+1 (85%), H-2→L+1 (3%), H-1→L+1 (9%)
3	649.302	1.910	0.622	H-2→L (15%), H-1→L (68%), H→L (8%)
4	610.910	2.030	0.416	H-2→L+1 (18%), H-1→L+1 (61%), H→L+1 (11%), H-1→L (6%)

5	535.916	2.314	0.169	H-2→L (75%), H-1→L (18%), H-3→L (4%)
6	512.458	2.419	0.755	H→L+2 (46%), H→L+3 (42%), H-1→L+1 (3%), H→L+4 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S17: Wavelength, excitation energy and oscillator strength of **ATTD8** in chloroform solvent at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	796.558	1.557	1.439	H→L (88%), H-1→L (8%)
2	688.419	1.801	0.308	H-1→L+1 (13%), H→L+1 (79%), H-2→L+1 (4%)
3	633.445	1.957	0.657	H-2→L (15%), H-1→L (68%), H→L (11%), H→L+1 (3%)
4	571.277	2.170	0.286	H-2→L+1 (17%), H-1→L+1 (58%), H→L+1 (17%), H-1→L (3%)
5	523.339	2.369	0.147	H-2→L (75%), H-1→L (17%), H-3→L (4%)
6	503.407	2.463	0.842	H→L+2 (87%), H→L+3 (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S18: Wave length λ (*nm*), excitation energy (*E*) and oscillator strength (*f*) of **ATTR1** in gaseous phase at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	695.057	1.784	3.007	H→L (95%), H-1→L+1 (4%)
2	579.041	2.141	0.001	H→L+1 (97%)
3	540.095	2.296	0.003	H-1→L (95%), H-2→L+1 (3%)
4	489.456	2.533	0.215	H-1→L+1 (92%), H→L (4%)
5	479.277	2.587	0.080	H-1→L+3 (14%), H→L+2 (81%)
6	470.368	2.636	0.001	H-1→L+2 (16%), H→L+3 (78%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S19: Wave length λ (*nm*), excitation energy (*E*) and oscillator strength (*f*) of **ATTD2** in gaseous phase at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	767.181	1.616	1.310	H→L (96%), H-1→L (2%)
2	600.204	2.066	1.118	H-1→L (85%), H-2→L (6%), H→L (3%), H→L+2 (3%)
3	526.293	2.356	0.265	H→L+1 (76%), H-2→L+1 (2%), H-1→L (3%), H-1→L+1 (9%), H→L+2 (5%)
4	511.359	2.425	0.109	H-2→L (83%), H-3→L (2%), H-1→L (7%), H→L+1 (4%)
5	481.548	2.575	0.501	H→L+2 (82%), H-2→L (5%), H→L+1 (3%), H→L+3 (2%)
6	454.338	2.729	0.027	H-2→L+1 (16%), H-1→L+1 (63%), H→L+1 (15%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S20: Wavelength, excitation energy and oscillator strength of **ATTD3** in gaseous phase at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	832.444	1.489	1.035	H→L (97%)
2	772.295	1.605	0.045	H→L+1 (92%), H-2→L+1 (2%), H-1→L+1 (5%)
3	634.417	1.954	0.627	H-1→L (57%), H-1→L+1 (17%), H-2→L (8%), H-2→L+1 (9%), H→L (2%), H→L+1 (3%)
4	616.960	2.010	0.679	H-2→L+1 (14%), H-1→L (27%), H-1→L+1 (46%), H→L+1 (5%), H→L+2 (2%)
5	555.410	2.232	0.164	H→L+2 (86%), H-2→L (3%), H-1→L (5%)
6	534.968	2.318	0.308	H-2→L (75%), H-1→L (8%), H-1→L+1 (4%), H→L+2 (6%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S21: Wavelength, excitation energy and oscillator strength of **ATTD4** in gaseous phase at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	765.098	1.621	1.215	H→L (94%), H-1→L (3%)
2	670.402	1.849	0.216	H-1→L+1 (11%), H→L+1 (81%), H-2→L+1 (3%)
3	603.711	2.054	0.827	H-2→L (10%), H-1→L (72%), H→L (5%), H→L+1 (5%), H→L+2 (3%)
4	555.087	2.234	0.436	H-2→L+1 (15%), H-1→L+1 (58%), H→L+1 (13%), H-1→L (8%), H→L+2 (2%)
5	507.010	2.445	0.317	H-2→L (73%), H-1→L (13%), H-3→L (2%), H→L+2 (9%)
6	484.749	2.558	0.488	H-2→L (10%), H→L+2 (79%), H-1→L+1 (4%), H→L+3 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S22: Wavelength, excitation energy and oscillator strength of **ATTD5** in gaseous phase at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	790.212	1.569	1.169	H→L (96%), H-1→L (2%)
2	702.102	1.766	0.170	H→L+1 (86%), H-2→L+1 (3%), H-1→L+1 (8%)
3	613.297	2.022	0.801	H-2→L (11%), H-1→L (72%), H-2→L+1 (3%), H-1→L+1 (3%), H→L (4%), H→L+1 (3%), H→L+2 (2%)
4	573.178	2.163	0.432	H-2→L+1 (17%), H-1→L (10%), H-1→L+1 (57%), H→L+1 (10%)
5	519.654	2.386	0.381	H-2→L (73%), H-1→L (13%), H→L+2 (8%)
6	488.608	2.538	0.487	H→L+2 (72%), H-2→L (8%), H-2→L+1 (3%), H-1→L+1 (8%), H→L+3 (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S23: Wavelength, excitation energy and oscillator strength of **ATTD6** in gaseous phase at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	822.122	1.508	1.041	H→L (97%), H-1→L (2%)
2	746.713	1.660	0.121	H→L+1 (90%), H-2→L+1 (2%), H-1→L+1 (6%)
3	630.161	1.968	0.735	H-2→L (10%), H-1→L (68%), H-2→L+1 (5%), H-1→L+1 (6%), H→L (3%), H→L+1 (3%)
4	600.902	2.063	0.552	H-2→L+1 (17%), H-1→L (15%), H-1→L+1 (56%), H→L+1 (7%)
5	533.908	2.322	0.462	H-2→L (74%), H-1→L (13%), H→L+2 (5%), H→L+3 (2%)
6	505.418	2.453	0.169	H-2→L+1 (55%), H-1→L+1 (29%), H-3→L+1 (3%), H→L+2 (8%), H→L+3 (3%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S24: Wavelength, excitation energy and oscillator strength of **ATTD7** in gaseous phase at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	822.940	1.507	1.073	H→L (97%)
2	753.245	1.646	0.134	H→L+1 (90%), H-2→L+1 (2%), H-1→L+1 (6%)
3	629.553	1.969	0.629	H-2→L (10%), H-1→L (63%), H-2→L+1 (7%), H-1→L+1 (9%), H→L (3%), H→L+1 (3%)
4	601.252	2.062	0.676	H-2→L+1 (15%), H-1→L (20%), H-1→L+1 (54%), H→L+1 (6%)
5	531.573	2.332	0.424	H-2→L (74%), H-1→L (13%), H-3→L (2%), H→L+2 (5%), H→L+3 (3%)
6	504.760	2.456	0.184	H-2→L+1 (52%), H-1→L+1 (28%), H→L+2 (10%), H-3→L+1 (3%), H→L+3 (4%)

MO=molecular orbital, H=HOMO, L=LUMO, f_{os}= oscillator strength, wavelength= λ (*nm*)

Table S25: Wavelength, excitation energy and oscillator strength of **ATTD8** in gaseous phase at M06/6-311G (d,p) level.

NO	DFT λ (*nm*)	*E*(*eV*)	f_{os}	MO contributions
1	757.850	1.636	1.234	H→L (94%), H-1→L (4%)
2	659.420	1.880	0.191	H-1→L+1 (12%), H→L+1 (80%), H-2→L+1 (4%)
3	601.427	2.062	0.892	H-2→L (10%), H-1→L (72%), H→L (5%), H→L+1 (5%), H→L+2 (3%)
4	550.747	2.251	0.360	H-2→L+1 (16%), H-1→L+1 (56%), H→L+1 (15%), H-1→L (7%)
5	507.861	2.441	0.347	H-2→L (72%), H-1→L (13%), H-3→L (2%), H→L+2 (9%)
6	484.389	2.560	0.497	H-2→L (10%), H→L+2 (78%), H-1→L+1 (4%), H→L+3 (3%)

Table S26: Natural bond orbitals analysis for the reference compound (**ATTR1**) with its representative values

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C23-C31	π	C33-C54	π*	33.74	0.3	0.091
C33-C54	π	C56-C57	π*	29.03	0.29	0.083
C34-C35	π	C47-O52	π*	24.88	0.3	0.08
C43-C44	π	C41-C42	π*	21.8	0.3	0.073
C9-C10	π	C11-C20	π*	20.07	0.3	0.071
C60-C61	π	C55-O58	π*	19.2	0.3	0.07
C11-C20	π	C9-C10	π*	18.5	0.32	0.071
C23-C31	π	C24-C25	π*	15.05	0.27	0.059
C24-C25	π	C11-C20	π*	13.26	0.31	0.059
C33-C54	π	C23-C31	π*	11.96	0.29	0.055
C27-C28	π	C90-C92	π*	11.64	0.31	0.055
C56-C57	π	C59-C64	π*	8.83	0.33	0.05
C37-C38	π	C34-C35	π*	8.06	0.33	0.047
C55-O58	π	C60-C61	π*	4.05	0.44	0.041
C47-O52	π	C34-C35	π*	3.59	0.42	0.038
C48-N49	π	C50-N51	π*	0.83	0.47	0.018
C67-N68	π	C69-N70	π*	0.78	0.48	0.017
C33-H53	σ	S26-C31	σ*	10.71	0.72	0.078
C25-S26	σ	C24-S101	σ*	8.72	0.86	0.077
C69-N70	σ	C57-C69	σ*	8.08	1.57	0.101
C67-N68	σ	C57-C67	σ*	7.97	1.58	0.101
C97-H100	σ	C89-S101	σ*	7.49	0.71	0.065
C11-C20	σ	C10-C21	σ*	6.76	1.18	0.08
C23-C24	σ	C24-C25	σ*	5.96	1.27	0.078
C40-C41	σ	C37-C42	σ*	5.77	1.19	0.074
C2-C3	σ	C3-C4	σ*	5.18	1.25	0.072
C10-C11	σ	C20-C25	σ*	4.94	1.24	0.07
C1-H7	σ	C5-C6	σ*	4.67	1.08	0.064
C93-H94	σ	C90-C92	σ*	4.3	0.54	0.046
C63-H105	σ	C61-C62	σ*	4.09	1.1	0.06
C64-H66	σ	C62-C63	σ*	3.92	1.11	0.059
C28-C29	σ	C27-C34	σ*	3.66	1.27	0.061
C11-H12	σ	C9-C10	σ*	3.08	1.11	0.052
C56-C57	σ	C59-C60	σ*	1.03	1.33	0.033
C89-C97	σ	C97-H100	σ*	0.57	1.08	0.022
S17-C20	σ	C11-C20	σ*	0.53	1.22	0.023
C67-N68	σ	C56-C57	σ*	0.5	1.65	0.026
S26	LP(2)	C24-C25	π*	28.61	0.25	0.078
S18	LP(2)	C14-C15	π*	22.8	0.27	0.071
S30	LP(2)	C27-C28	π*	19.08	0.27	0.066
O52	LP(2)	C43-C47	σ*	20.79	0.76	0.114
O52	LP(2)	C35-C47	σ*	18.06	0.76	0.106
S30	LP(1)	C27-C34	σ*	0.52	1.23	0.023

Donor(*i*)	Type	Acceptor(*j*)	Type	*E*(2) [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i*,*j*) [*a.u*]
C27-C28	π	C33-C34	π*	34.84	0.3	0.092
C33-C34	π	C36-C37	π*	29.88	0.29	0.084
C89-C93	π	C86-C87	π*	25.67	0.3	0.079
C39-C40	π	C41-C42	π*	23.5	0.3	0.075
C107-C108	π	C109-C112	π*	22.55	0.31	0.074
C86-C87	π	C89-C93	π*	20.98	0.29	0.07
C11-C20	π	C9-C10	π*	19.65	0.32	0.074
C5-C6	π	C1-C2	π*	18.84	0.3	0.069
C23-C31	π	C24-C25	π*	17.02	0.29	0.067
C29-C32	π	C14-C15	π*	13.21	0.31	0.059
C23-C31	π	C86-C87	π*	10.52	0.32	0.054
C36-C37	π	C41-C42	π*	8.12	0.33	0.048
C46-O51	π	C41-C42	π*	4.03	0.43	0.041
C46-O51	π	C33-C34	π*	3.56	0.42	0.038
C47-N48	π	C49-N50	π*	0.84	0.47	0.018
C49-N50	π	C47-N48	π*	0.79	0.48	0.017
C107-C108	π	C97-C99	π*	0.76	0.3	0.014
C33-H35	σ	C27-S30	σ*	10.85	0.72	0.079
C25-S26	σ	C24-S82	σ*	9.2	0.86	0.079
S30-C32	σ	C29-S83	σ*	8.7	0.86	0.077
C2-C3	σ	S18-C19	σ*	7.85	0.89	0.075
C68-H69	σ	C70-S82	σ*	6.9	0.72	0.063
C23-C24	σ	C20-C25	σ*	6.11	1.21	0.077
C14-C15	σ	C15-C32	σ*	5.84	1.27	0.077
S30-C32	σ	C15-S18	σ*	5.74	0.85	0.062
C68-C70	σ	C23-C31	σ*	5.19	1.35	0.075
C70-S82	σ	C24-C25	σ*	4.98	1.24	0.07
C99-H103	σ	C97-C98	σ*	4.84	1.1	0.065
C109-H113	σ	C107-C108	σ*	4.64	1.11	0.064
C97-C98	σ	C98-C100	σ*	3.96	1.31	0.065
C38-H85	σ	C42-C43	σ*	3.79	1.13	0.058
C24-S82	σ	C70-C78	σ*	2.98	1.12	0.052
C24-C25	σ	C11-C20	σ*	2.37	1.33	0.05
C34-C46	σ	C46-O51	σ*	1.99	1.25	0.045
C5-C21	σ	C9-S17	σ*	0.61	0.83	0.02
C123-H126	σ	C104-O118	σ*	0.54	0.91	0.02
C73-S83	σ	C28-C29	σ*	0.51	1.2	0.022
O118	LP(2)	C102-C104	π*	32.47	0.36	0.103
S83	LP(2)	C71-C73	π*	24.45	0.29	0.076
S30	LP(2)	C33-C34	π*	0.52	0.28	0.011
O51	LP(2)	C42-C46	σ*	20.86	0.76	0.114
N50	LP(1)	C37-C49	σ*	12.49	1.05	0.102
S83	LP(1)	S18-C19	σ*	0.52	0.89	0.019

Table S27: Natural bond orbitals analysis for **ATTD2** with its representative values

Table S28: Natural bond orbitals analysis for **ATTD3** with its representative values

Donor(*i*)	Type	Acceptor(*j*)	Type	*E*(2) [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i*,*j*) [*a.u*]
C27-C28	π	C33-C34	π*	36.23	0.3	0.093
C33-C34	π	C36-C37	π*	28.21	0.29	0.081
C83-C87	π	C80-C81	π*	25.61	0.3	0.079
C80-C81	π	C82-C85	π*	22.59	0.3	0.074
C123-C125	π	C121-C126	π*	20.37	0.31	0.072
C92-C94	π	C91-C93	π*	19.33	0.3	0.07
C40-C41	π	C36-C37	π*	18.95	0.32	0.071
C14-C15	π	C13-C19	π*	17.99	0.32	0.07
C11-C20	π	C24-C25	π*	15.62	0.29	0.065
C29-C32	π	C14-C15	π*	12.96	0.31	0.058
C23-C31	π	C80-C81	π*	10.72	0.32	0.054
C36-C37	π	C33-C34	π*	7.76	0.33	0.047
N131-O132	π	C121-C126	π*	2.92	0.52	0.038
C36-C37	π	C43-N44	π*	1.16	0.41	0.02
C43-N44	π	C45-N46	π*	0.85	0.47	0.018
C45-N46	π	C43-N44	π*	0.79	0.47	0.017
C101-C102	π	C91-C93	π*	0.76	0.3	0.014
C33-H35	σ	C27-S30	σ*	10.77	0.72	0.079
C25-S26	σ	C24-S78	σ*	9.19	0.86	0.079
S30-C32	σ	C29-S79	σ*	8.64	0.86	0.077
C2-C3	σ	S18-C19	σ*	7.86	0.89	0.075
C15-C32	σ	C29-C32	σ*	6.87	1.31	0.085
C23-C24	σ	C20-C25	σ*	6.08	1.21	0.077
C34-C42	σ	C41-S127	σ*	5.88	0.89	0.065
C28-C29	σ	C15-C32	σ*	5.62	1.25	0.075
C13-C19	σ	C3-C4	σ*	5.05	1.29	0.072
C66-S78	σ	C24-C25	σ*	4.97	1.24	0.07
C66-S78	σ	C64-H65	σ*	4.53	1.06	0.062
C92-H95	σ	C94-C98	σ*	4.07	1.09	0.06
C38-C121	σ	C126-N131	σ*	3.98	1.03	0.058
C29-S79	σ	C69-C70	σ*	3.18	1.13	0.054
C67-H68	σ	C28-C29	σ*	2.86	1.07	0.049
C104-C108	σ	C102-H105	σ*	2.28	1.14	0.046
C21-C60	σ	C5-C21	σ*	1.99	1.05	0.041
C22-C48	σ	C48-H50	σ*	0.6	1.01	0.022
C117-H120	σ	C98-O112	σ*	0.53	0.91	0.02
C69-S79	σ	C28-C29	σ*	0.51	1.2	0.022
O112	LP(2)	C96-C98	π*	32.44	0.36	0.103
S26	LP(2)	C24-C25	π*	22.66	0.27	0.071
S30	LP(2)	C33-C34	π*	0.54	0.28	0.011
O47	LP(2)	C41-C42	σ*	22.65	0.74	0.117
N46	LP(1)	C37-C45	σ*	12.59	1.04	0.102
O129	LP(2)	C125-C126	σ*	0.5	0.84	0.019

Table S29: Natural bond orbitals analysis for **ATTD4** with its representative values.

Donor(*i*)	Type	Acceptor(*j*)	Type	*E*(2) [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i*,*j*) [*a.u*]
C27-C28	π	C33-C34	π*	34.1	0.3	0.091
C83-C87	π	C80-C81	π*	25.81	0.3	0.079
C3-C4	π	C5-C6	π*	24.76	0.3	0.077
C80-C81	π	C82-C85	π*	22.7	0.3	0.074
C40-C41	π	C42-O47	π*	21.28	0.33	0.075
C39-C123	π	C40-C41	π*	19.5	0.28	0.067
C104-C108	π	C103-C106	π*	18.41	0.31	0.068
C82-C85	π	C80-C81	π*	18.07	0.3	0.068
C5-C6	π	C9-C10	π*	16.18	0.29	0.062
C9-C10	π	C5-C6	π*	15.75	0.32	0.066
C24-C25	π	C11-C20	π*	14.57	0.32	0.064
C27-C28	π	C67-C69	π*	11.57	0.31	0.055
C36-C37	π	C33-C34	π*	7.79	0.33	0.047
C42-O47	π	C40-C41	π*	4.24	0.41	0.041
C36-C37	π	C43-N44	π*	1.17	0.41	0.021
C43-N44	π	C45-N46	π*	0.84	0.47	0.018
C45-N46	π	C43-N44	π*	0.77	0.48	0.017
C33-H35	σ	C27-S30	σ*	10.58	0.72	0.078
C25-S26	σ	C24-S78	σ*	9.21	0.86	0.079
C37-C45	σ	C45-N46	σ*	8.16	1.61	0.103
C20-C25	σ	C24-C25	σ*	7.76	1.33	0.091
C27-C33	σ	C33-C34	σ*	6.89	1.34	0.086
C23-C24	σ	C20-C25	σ*	6.08	1.21	0.077
C28-C29	σ	C15-C32	σ*	5.68	1.24	0.075
C64-C66	σ	C23-C31	σ*	5.19	1.35	0.075
C66-S78	σ	C24-C25	σ*	4.97	1.24	0.07
C82-H86	σ	C80-C81	σ*	4.35	1.09	0.062
C96-H100	σ	C94-C98	σ*	4.04	1.1	0.06
S18-C19	σ	C13-C22	σ*	3.69	1.15	0.059
C14-H16	σ	C13-C19	σ*	3.09	1.11	0.052
C125-C126	σ	C123-H124	σ*	2.02	1.17	0.044
C10-C21	σ	C60-H63	σ*	1.49	1.01	0.035
C33-C34	σ	C41-C42	σ*	1.06	1.19	0.032
C23-C24	σ	C25-S26	σ*	0.56	0.88	0.02
C117-H120	σ	C98-O112	σ*	0.54	0.91	0.02
S17-C20	σ	C10-C21	σ*	0.51	1.11	0.021
O111	LP(2)	C104-C108	π*	32.59	0.36	0.103
S78	LP(2)	C64-C66	π*	22.01	0.29	0.072
S30	LP(2)	C33-C34	π*	0.5	0.28	0.011
O47	LP(2)	C41-C42	σ*	22.21	0.74	0.116
O112	LP(2)	C117-H119	σ*	6.08	0.69	0.06
Cl128	LP(2)	C38-C121	σ*	0.5	0.9	0.019

Table S30: Natural bond orbitals analysis for **ATTD5** with its representative values

Donor(*i*)	Type	Acceptor(*j*)	Type	*E*(2) [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i*,*j*) [*a.u*]
C27-C28	π	C33-C34	π*	35.22	0.3	0.093
C33-C34	π	C36-C37	π*	27.35	0.29	0.08
C85-C87	π	C80-C82	π*	25.89	0.3	0.079
C96-C98	π	C91-C93	π*	24.45	0.3	0.078
C29-C32	π	C27-C28	π*	23.12	0.31	0.08
C80-C82	π	C81-C83	π*	22.85	0.3	0.074
C92-C94	π	C96-C98	π*	22.72	0.29	0.075
C101-C102	π	C103-C106	π*	22.61	0.31	0.074
C103-C106	π	C104-C108	π*	22.29	0.3	0.075
C81-C83	π	C85-C87	π*	21.72	0.3	0.074
C38-C39	π	C123-C125	π*	19.41	0.31	0.071
C64-C66	π	C23-C31	π*	18.23	0.32	0.074
C23-C31	π	C24-C25	π*	17.07	0.29	0.067
C36-C37	π	C40-C41	π*	9.09	0.31	0.049
C42-O47	π	C40-C41	π*	4.28	0.41	0.041
C101-C102	π	C91-C93	π*	0.84	0.3	0.014
C45-N46	π	C43-N44	π*	0.78	0.48	0.017
C33-H35	σ	C27-S30	σ*	10.72	0.72	0.078
C37-C43	σ	C43-N44	σ*	8.41	1.61	0.104
C20-C25	σ	C24-C25	σ*	7.76	1.33	0.091
C29-C32	σ	C15-C32	σ*	6.83	1.3	0.084
C123-C125	σ	C125-C126	σ*	6.19	1.27	0.079
C3-C4	σ	C2-C3	σ*	5.77	1.27	0.076
C2-C22	σ	C13-C14	σ*	5.53	1.19	0.073
C1-C6	σ	C5-C6	σ*	5.51	1.27	0.075
C4-H8	σ	C5-C6	σ*	5.15	1.08	0.067
C5-C6	σ	C1-C6	σ*	5.04	1.25	0.071
C93-H97	σ	C91-C92	σ*	4.84	1.1	0.065
C91-C92	σ	C91-C93	σ*	4.76	1.3	0.07
C93-C96	σ	N90-C91	σ*	4.63	1.13	0.065
C94-C98	σ	C96-C98	σ*	4.8	1.28	0.07
C103-C106	σ	N90-C101	σ*	4.5	1.14	0.064
O111-C113	σ	C106-C108	σ*	3.08	1.42	0.059
N90-C91	σ	C87-N90	σ*	2.58	1.21	0.05
C21-C60	σ	C60-H63	σ*	0.61	1.01	0.022
C117-H120	σ	C98-O112	σ*	0.54	0.91	0.02
C45-N46	σ	C36-C37	σ*	0.5	1.64	0.026
O112	LP(2)	C96-C98	π*	32.51	0.36	0.103
S17	LP(2)	C11-C20	π*	23.61	0.28	0.073
F134	LP(2)	C123-C125	π*	0.52	0.48	0.015
O47	LP(2)	C41-C42	σ*	22.37	0.74	0.117
O47	LP(1)	S30-C32	σ*	1.21	0.93	0.03
F130	LP(2)	C125-C126	σ*	0.51	1	0.02

Table S31: Natural bond orbitals analysis for **ATTD6** with its representative values.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C27-C28	π	C33-C34	π*	36.16	0.3	0.093
C33-C34	π	C36-C37	π*	28.25	0.29	0.081
C33-C34	π	C42-O47	π*	26.76	0.3	0.081
C104-C108	π	C101-C102	π*	24.11	0.3	0.077
C91-C93	π	C92-C94	π*	22.59	0.31	0.074
C81-C83	π	C85-C87	π*	21.69	0.3	0.074
C40-C41	π	C42-O47	π*	19.97	0.33	0.073
C85-C87	π	C81-C83	π*	18.89	0.3	0.068
C24-C25	π	C11-C20	π*	14.33	0.32	0.063
C29-C32	π	C14-C15	π*	12.97	0.31	0.058
C23-C31	π	C80-C82	π*	10.12	0.32	0.053
C36-C37	π	C40-C41	π*	9.14	0.31	0.049
C36-C37	π	C33-C34	π*	7.75	0.33	0.047
C42-O47	π	C40-C41	π*	4.3	0.41	0.041
C36-C37	π	C43-N44	π*	1.19	0.41	0.021
C43-N44	π	C45-N46	π*	0.82	0.47	0.018
C101-C102	π	C91-C93	π*	0.77	0.3	0.014
C33-H35	σ	C27-S30	σ*	10.74	0.72	0.079
C25-S26	σ	C24-S78	σ*	9.2	0.86	0.079
S30-C32	σ	C29-S79	σ*	8.63	0.86	0.077
C24-C25	σ	C20-C25	σ*	7.68	1.29	0.089
C27-C33	σ	C33-C34	σ*	6.85	1.34	0.085
C23-C24	σ	C20-C25	σ*	6.07	1.21	0.077
C34-C42	σ	C41-S127	σ*	5.91	0.88	0.065
C67-C69	σ	C27-C28	σ*	5.71	1.29	0.077
C121-H122	σ	C38-C39	σ*	4.99	1.06	0.065
C102-H105	σ	C101-C103	σ*	4.81	1.1	0.065
C28-C67	σ	C67-C69	σ*	4.22	1.3	0.066
C36-C40	σ	C33-C34	σ*	3.97	1.28	0.064
C52-H53	σ	C13-C22	σ*	3.73	0.95	0.053
C24-S78	σ	C66-C74	σ*	2.98	1.12	0.052
C96-C98	σ	C94-H99	σ*	1.99	1.14	0.043
N90-C91	σ	C93-C96	σ*	1.49	1.36	0.04
S18-C19	σ	C13-C19	σ*	1.02	1.28	0.032
C23-C24	σ	C25-S26	σ*	0.56	0.88	0.02
S17-C20	σ	C10-C21	σ*	0.51	1.11	0.021
C45-N46	σ	C36-C37	σ*	0.5	1.64	0.026
O112	LP(2)	C96-C98	π*	32.44	0.36	0.103
S79	LP(2)	C67-C69	π*	24.62	0.29	0.076
S30	LP(2)	C33-C34	π*	0.53	0.28	0.011
O131	LP(1)	S128-O129	σ*	2.68	1.02	0.048
O129	LP(1)	S128-O130	σ*	1.61	1.17	0.04
O136	LP(2)	C123-C125	σ*	0.5	0.97	0.02

Table S32: Natural bond orbitals analysis for **ATTD7** with its representative values.

Donor(*i*)	**Type**	**Acceptor(*j*)**	**Type**	***E*(2) [*kcal/mol*]**	***E*(*j*)-*E*(*i*) [*a.u*]**	***F*(*i*,*j*) [*a.u*]**
C27-C28	π	C33-C34	π*	35.93	0.3	0.093
C33-C34	π	C36-C37	π*	27.92	0.29	0.081
C33-C34	π	C42-O47	π*	26.79	0.3	0.081
C39-C123	π	C125-C126	π*	24.52	0.27	0.075
C29-C32	π	C27-C28	π*	23.38	0.31	0.081
C92-C94	π	C96-C98	π*	22.6	0.29	0.075
C3-C4	π	C1-C2	π*	21.08	0.3	0.073
C92-C94	π	C91-C93	π*	19.33	0.3	0.07
C23-C31	π	C80-C81	π*	10.39	0.32	0.054
C36-C37	π	C40-C41	π*	9.03	0.31	0.049
C36-C37	π	C33-C34	π*	7.77	0.33	0.047
C42-O47	π	C40-C41	π*	4.32	0.41	0.041
C42-O47	π	C33-C34	π*	3.47	0.43	0.038
C36-C37	π	C43-N44	π*	1.09	0.41	0.02
C67-C69	π	C67-C69	π*	0.91	0.32	0.016
C43-N44	π	C45-N46	π*	0.82	0.47	0.018
C45-N46	π	C43-N44	π*	0.76	0.47	0.017
C33-H35	σ	C27-S30	σ*	10.72	0.72	0.078
C25-S26	σ	C24-S78	σ*	9.2	0.86	0.079
C126-C130	σ	C130-N131	σ*	8.93	1.62	0.108
C2-C3	σ	S18-C19	σ*	7.87	0.89	0.075
C15-C32	σ	C29-C32	σ*	6.9	1.32	0.085
C38-C39	σ	C36-C40	σ*	6.39	1.18	0.078
C36-C37	σ	C37-C45	σ*	6.01	1.27	0.078
S30-C32	σ	C15-S18	σ*	5.72	0.85	0.062
C9-C10	σ	C1-C6	σ*	5.08	1.29	0.072
C66-S78	σ	C24-C25	σ*	4.97	1.24	0.07
S17-C20	σ	C11-H12	σ*	3.89	1.06	0.058
C85-C87	σ	N90-C91	σ*	3.56	1.13	0.057
C29-S79	σ	S30-C32	σ*	3.08	0.89	0.047
C125-C128	σ	C39-C123	σ*	2.99	1.3	0.056
C5-C21	σ	C3-C4	σ*	2.06	1.19	0.044
C10-C21	σ	C21-C60	σ*	1.73	1.01	0.038
C102-H105	σ	N90-C101	σ*	1.01	0.94	0.028
C66-S78	σ	C23-C24	σ*	0.58	1.17	0.023
C117-H120	σ	C98-O112	σ*	0.54	0.91	0.02
C69-S79	σ	C28-C29	σ*	0.51	1.2	0.022
N90	LP(1)	C83-C87	π*	32.73	0.29	0.091
S127	LP(2)	C38-C121	π*	23.85	0.27	0.072
S30	LP(2)	C33-C34	π*	0.53	0.28	0.011
O47	LP(2)	C41-C42	σ*	22.62	0.74	0.117
N90	LP(1)	C91-C93	σ*	3.88	0.85	0.055

S30	LP(1)	C27-C33	σ*	0.51	1.24	0.022

Table S33: Natural bond orbitals analysis for **ATTD8** with its representative values.

Donor(*i*)	Type	Acceptor(*j*)	Type	*E*(2) [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i*,*j*) [*a.u*]
C27-C28	π	C33-C34	π*	34.19	0.3	0.092
C33-C34	π	C36-C37	π*	26.56	0.29	0.079
C83-C87	π	C80-C81	π*	25.51	0.3	0.079
C125-C126	π	C38-C121	π*	24.92	0.28	0.074
C5-C6	π	C3-C4	π*	23.89	0.29	0.074
C1-C2	π	C5-C6	π*	22.77	0.3	0.076
C80-C81	π	C83-C87	π*	21.04	0.29	0.07
C13-C19	π	C14-C15	π*	20.6	0.29	0.072
C1-C2	π	C3-C4	π*	19.34	0.3	0.07
C96-C98	π	C92-C94	π*	18.63	0.31	0.068
C23-C31	π	C24-C25	π*	17.04	0.29	0.067
C40-C41	π	C39-C123	π*	16.6	0.33	0.069
C24-C25	π	C23-C31	π*	15.34	0.33	0.067
C36-C37	π	C33-C34	π*	7.82	0.33	0.047
C131-O132	π	C125-C126	π*	1.32	0.44	0.024
C36-C37	π	C43-N44	π*	0.98	0.41	0.019
C101-C102	π	C91-C93	π*	0.72	0.3	0.013
C33-H35	σ	C27-S30	σ*	10.61	0.72	0.078
C25-S26	σ	C24-S78	σ*	9.2	0.86	0.079
S30-C32	σ	C29-S79	σ*	8.73	0.86	0.077
C2-C3	σ	S18-C19	σ*	7.84	0.9	0.075
C15-C32	σ	C29-C32	σ*	6.91	1.32	0.085
C27-S30	σ	C28-C67	σ*	5.73	1.2	0.074
C64-C66	σ	C23-C31	σ*	5.19	1.35	0.075
C121-H122	σ	C38-C39	σ*	4.98	1.05	0.065
C93-H97	σ	C91-C92	σ*	4.81	1.1	0.065
C37-C43	σ	C34-C36	σ*	3.95	1.24	0.063
C9-C10	σ	C11-H12	σ*	3.69	1.11	0.057
C80-C82	σ	S26-C31	σ*	3.34	0.91	0.049
C38-C121	σ	C126-C131	σ*	2.98	1.18	0.054
C80-C82	σ	C85-H89	σ*	2.33	1.12	0.046
C96-C98	σ	C94-H99	σ*	2.01	1.14	0.043
C20-C25	σ	C23-C24	σ*	1.77	1.25	0.042
C36-C40	σ	C38-C39	σ*	1.01	1.2	0.031
C23-C24	σ	C25-S26	σ*	0.56	0.88	0.02
C117-H120	σ	C98-O112	σ*	0.54	0.91	0.02
C123-H124	σ	C125-C128	σ*	0.5	0.96	0.02
O130	LP(2)	C128-O129	π*	50.66	0.37	0.124
S17	LP(2)	C9-C10	π*	23.76	0.29	0.075
S30	LP(2)	C33-C34	π*	0.5	0.28	0.011
O132	LP(2)	C131-O133	σ*	33.13	0.68	0.135
O133	LP(2)	C138-H139	σ*	5.28	0.71	0.058

S79	LP(1)	S18-C19	σ*	0.51	0.89	0.019

Table S34: Dipole moment (*u*) and major contributing tensors (*D*) of the studied compounds.

Compounds	u_x	u_y	u_z	u_{total}

ATTR1	-0.0005	-0.0001	0.4618	0.46
ATTD2	-18.1919	1.1142	2.3406	18.38
ATTD3	27.2462	0.6546	0.7476	27.26
ATTD4	19.2814	-1.3926	0.2677	19.33
ATTD5	22.8245	-0.2264	0.2871	22.83
ATTD6	-24.6976	0.6917	1.9786	24.79
ATTD7	-28.0619	1.3336	-1.5738	28.14
ATTD8	-16.4007	1.2622	-1.2087	16.49

Table S35: Linear polarizabilities and major contributing tensors (*esu*) of the compounds (**ATTR1** and **ATTD2-ATTD8**).

Compounds	$\alpha_{xx} \times 10^{-22}$	$\alpha_{yy} \times 10^{-22}$	$\alpha_{zz} \times 10^{-22}$	$\langle\alpha\rangle \times 10^{-22}$
ATTR1	6.30	2.19	0.65	3.05
ATTD2	5.84	2.21	0.87	2.97
ATTD3	6.24	2.35	0.99	3.19
ATTD4	5.98	2.37	0.91	3.09
ATTD5	6.05	2.36	0.92	3.11
ATTD6	6.23	2.39	1.02	3.21
ATTD7	6.30	2.39	0.92	3.20
ATTD8	5.98	2.41	0.99	3.13

Table S36: The calculated first hyperpolarizability (β_{tot}) along its major contributing tensors (*esu*) of **ATTR1** and **ATTD2-ATTD8**.

Systems	**ATTR1**	**ATTD2**	**ATTD3**	**ATTD4**	**ATTD5**	**ATTD6**	**ATTD7**	**ATTD8**
$\beta_{xxx}\times10^{-27}$	-0.0001	-6.97	8.06	5.98	6.70	-7.45	-7.74	-5.86
$\beta_{xxy}\times10^{-28}$	-0.0003	4.36	-7.50	-6.91	-8.97	-9.74	-7.41	-7.16
$\beta_{xyy}\times10^{-29}$	0.0003	-0.69	12.4	1.10	8.80	-12.0	-7.24	-3.83
$\beta_{yyy}\times10^{-30}$	0.001	-9.90	29.8	-16.4	-3.27	5.04	15.9	-8.46
$\beta_{xxz}\times10^{-29}$	5.00	-1.36	-17.0	-5.74	-15.8	14.5	6.51	13.6
$\beta_{yyz}\times10^{-30}$	3.60	-4.25	-11.3	-4.92	-1.47	9.83	5.61	3.97
$\beta_{xzz}\times10^{-30}$	0.001	4.31	6.97	-3.37	2.56	-4.96	2.92	-9.69
$\beta_{yzz}\times10^{-31}$	0.003	-1.84	8.08	3.41	-5.90	2.95	4.71	-0.099
$\beta_{zzz}\times10^{-30}$	-0.31	-1.40	-1.07	-1.15	-1.30	0.614	1.12	0.956
$\beta_{tot}\times10^{-27}$	0.05	6.98	8.23	6.03	6.86	7.64	7.84	5.96

Table S37: Second hyper-polarizabilities and major contributing tensors (*esu*) of the studied compounds.

Compounds	$\gamma_x\times10^{-31}$	$\gamma_y\times10^{-33}$	$\gamma_z\times10^{-35}$	$\langle\gamma\rangle\times10^{-31}$
ATTR1	0.72	0.10	0.43	0.72
ATTD2	1.28	0.83	0.96	1.29
ATTD3	1.63	2.88	12.7	1.66
ATTD4	1.08	1.69	0.98	1.10
ATTD5	1.21	2.48	6.69	1.24
ATTD6	1.42	3.01	9.51	1.45
ATTD7	1.47	2.21	1.10	1.49
ATTD8	1.06	1.89	10.2	1.08

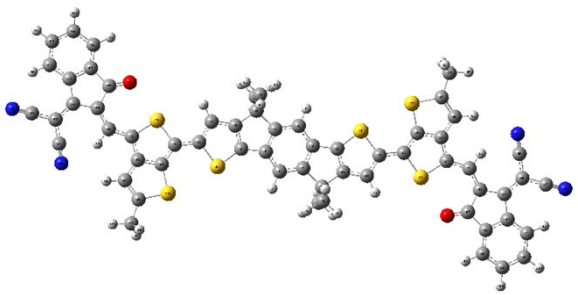
Table S38: The IUPAC names and abbreviations of investigated compounds

Compound	IUPAC name
ATTD2	(Z)-2-(2-((6-(7-(4-(4-(bis(4-methoxyphenyl)amino)phenyl)-2-methylthieno[3,4-b]thiophen-6-yl)-4,4,9,9-tetramethyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophen-2-yl)-2-methylthieno[3,4-b]thiophen-4-yl)methylene)-3-oxo-2,3-dihydro-1*H*-inden-1-ylidene)malononitrile
ATTD3	(Z)-2-(2-((6-(7-(4-(4-(bis(4-methoxyphenyl)amino)phenyl)-2-methylthieno[3,4-b]thiophen-6-yl)-4,4,9,9-tetramethyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophen-2-yl)-2-methylthieno[3,4-b]thiophen-4-yl)methylene)-6,7-dinitro-3-oxo-2,3-dihydro-1*H*-benzo[b]cyclopenta[d]thiophen-1-ylidene)malononitrile
ATTD4	(Z)-2-(2-((6-(7-(4-(4-(bis(4-methoxyphenyl)amino)phenyl)-2-methylthieno[3,4-b]thiophen-6-yl)-4,4,9,9-tetramethyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophen-2-yl)-2-methylthieno[3,4-b]thiophen-4-yl)methylene)-6,7-dichloro-3-oxo-2,3-dihydro-1*H*-benzo[b]cyclopenta[d]thiophen-1-ylidene)malononitrile
ATTD5	(Z)-2-(2-((6-(7-(4-(4-(bis(4-methoxyphenyl)amino)phenyl)-2-methylthieno[3,4-b]thiophen-6-yl)-4,4,9,9-tetramethyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophen-2-yl)-2-methylthieno[3,4-b]thiophen-4-yl)methylene)-3-oxo-6,7-bis(trifluoromethyl)-2,3-dihydro-1*H*-benzo[b]cyclopenta[d]thiophen-1-ylidene)malononitrile
ATTD6	(Z)-2-((6-(7-(4-(4-(bis(4-methoxyphenyl)amino)phenyl)-2-methylthieno[3,4-b]thiophen-6-yl)-4,4,9,9-tetramethyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophen-2-yl)-2-methylthieno[3,4-b]thiophen-4-yl)methylene)-1-(dicyanomethylene)-3-oxo-2,3-dihydro-1*H*-benzo[b]cyclopenta[d]thiophene-6,7-disulfonic acid
ATTD7	Z)-2-((6-(7-(4-(4-(bis(4-methoxyphenyl)amino)phenyl)-2-methylthieno[3,4-b]thiophen-6-yl)-4,4,9,9-tetramethyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophen-2-yl)-2-methylthieno[3,4-b]thiophen-4-yl)methylene)-1-(dicyanomethylene)-3-oxo-2,3-dihydro-1*H*-benzo[b]cyclopenta[d]thiophene-6,7-dicarbonitrile
ATTD8	dimethyl(Z)-2-((6-(7-(4-(4-(bis(4-methoxyphenyl)amino)phenyl)-2-methylthieno[3,4-b]thiophen-6-yl)-4,4,9,9-tetramethyl-4,9-dihydro-s-indaceno[1,2-b:5,6-b']dithiophen-2-yl)-2-methylthieno[3,4-b]thiophen-4-yl)methylene)-1-(dicyanomethylene)-3-oxo-2,3-dihydro-1*H*-benzo[b]cyclopenta[d]thiophene-6,7-dicarboxylate

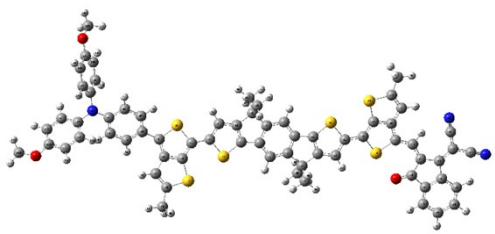
Table S39: Representative values of NBOs study for the entitled compounds (**ATTR1** and **ATTD2-ATTD8**).

Compounds	Donor(*i*)	Type	Acceptor(*j*)	Type	*E*(2) [*kcal/mol*]	*E*(*j*)-*E*(*i*) [*a.u*]	*F*(*i*,*j*) [*a.u*]
ATTR1	C23-C31	π	C33-C54	π*	33.74	0.3	0.091
	C67-N68	π	C69-N70	π*	0.78	0.48	0.017
	C33-H53	σ	S26-C31	σ*	10.71	0.72	0.078
	C67-N68	σ	C56-C57	σ*	0.5	1.65	0.026
	S26	LP(2)	C24-C25	π*	28.61	0.25	0.078

	O52	LP(2)	C43-C47	σ*	20.79	0.76	0.114
ATTD2	C27-C28	π	C33-C34	π*	34.84	0.3	0.092
	C107-C108	π	C97-C99	π*	0.76	0.3	0.014
	C33-H35	σ	C27-S30	σ*	10.85	0.72	0.079
	C73-S83	σ	C28-C29	σ*	0.51	1.2	0.022
	O118	LP(2)	C102-C104	π*	32.47	0.36	0.103
	O51	LP(2)	C42-C46	σ*	20.86	0.76	0.114
ATTD3	C27-C28	π	C33-C34	π*	36.23	0.3	0.093
	C101-C102	π	C91-C93	π*	0.76	0.3	0.014
	C33-H35	σ	C27-S30	σ*	10.77	0.72	0.079
	C69-S79	σ	C28-C29	σ*	0.51	1.2	0.022
	O112	LP(2)	C96-C98	π*	32.44	0.36	0.103
	O47	LP(2)	C41-C42	σ*	22.65	0.74	0.117
ATTD4	C27-C28	π	C33-C34	π*	34.1	0.3	0.091
	C45-N46	π	C43-N44	π*	0.77	0.48	0.017
	C33-H35	σ	C27-S30	σ*	10.58	0.72	0.078
	S17-C20	σ	C10-C21	σ*	0.51	1.11	0.021
	O111	LP(2)	C104-C108	π*	32.59	0.36	0.103
	O47	LP(2)	C41-C42	σ*	22.21	0.74	0.116
ATTD5	C27-C28	π	C33-C34	π*	35.22	0.3	0.093
	C45-N46	π	C43-N44	π*	0.78	0.48	0.017
	C33-H35	σ	C27-S30	σ*	10.72	0.72	0.078
	C45-N46	σ	C36-C37	σ*	0.5	1.64	0.026
	O112	LP(2)	C96-C98	π*	32.51	0.36	0.103
	O47	LP(2)	C41-C42	σ*	22.37	0.74	0.117
ATTD6	C27-C28	π	C33-C34	π*	36.16	0.3	0.093
	C101-C102	π	C91-C93	π*	0.77	0.3	0.014
	C33-H35	σ	C27-S30	σ*	10.74	0.72	0.079
	C45-N46	σ	C36-C37	σ*	0.5	1.64	0.026
	O112	LP(2)	C96-C98	π*	32.44	0.36	0.103
	O131	LP(1)	S128-O129	σ*	2.68	1.02	0.048
ATTD7	C27-C28	π	C33-C34	π*	35.93	0.3	0.093
	C45-N46	π	C43-N44	π*	0.76	0.47	0.017
	C33-H35	σ	C27-S30	σ*	10.72	0.72	0.078
	C69-S79	σ	C28-C29	σ*	0.51	1.2	0.022
	N90	LP(1)	C83-C87	π*	32.73	0.29	0.091
	O47	LP(2)	C41-C42	σ*	22.62	0.74	0.117
ATTD8	C27-C28	π	C33-C34	π*	34.19	0.3	0.092
	C101-C102	π	C91-C93	π*	0.72	0.3	0.013
	C33-H35	σ	C27-S30	σ*	10.61	0.72	0.078
	C123-H124	σ	125-C128	σ*	0.5	0.96	0.02
	O130	LP(2)	C128-O129	π*	50.66	0.37	0.124
	O132	LP(2)	C131-O133	σ*	33.13	0.68	0.135



ATTR1



ATTD2

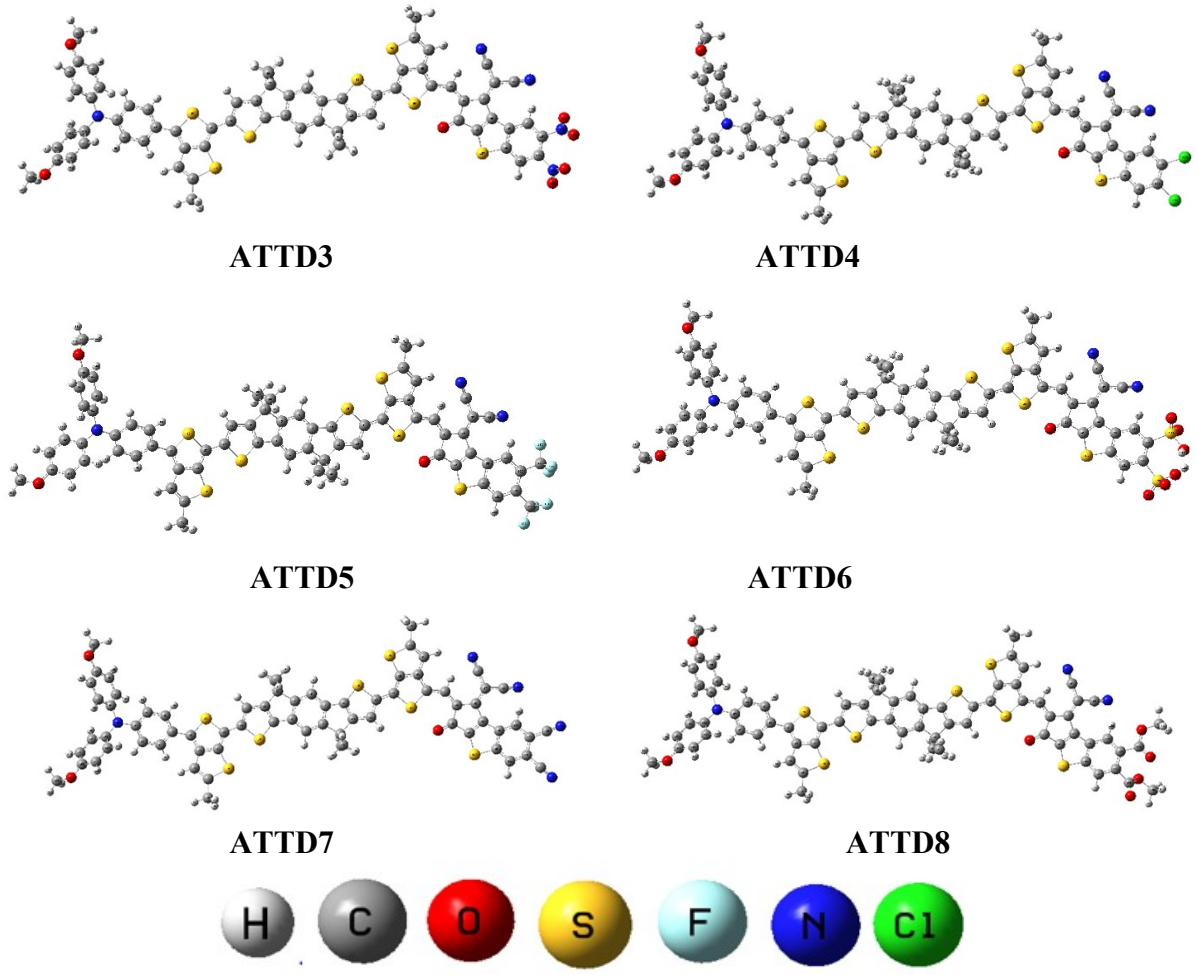
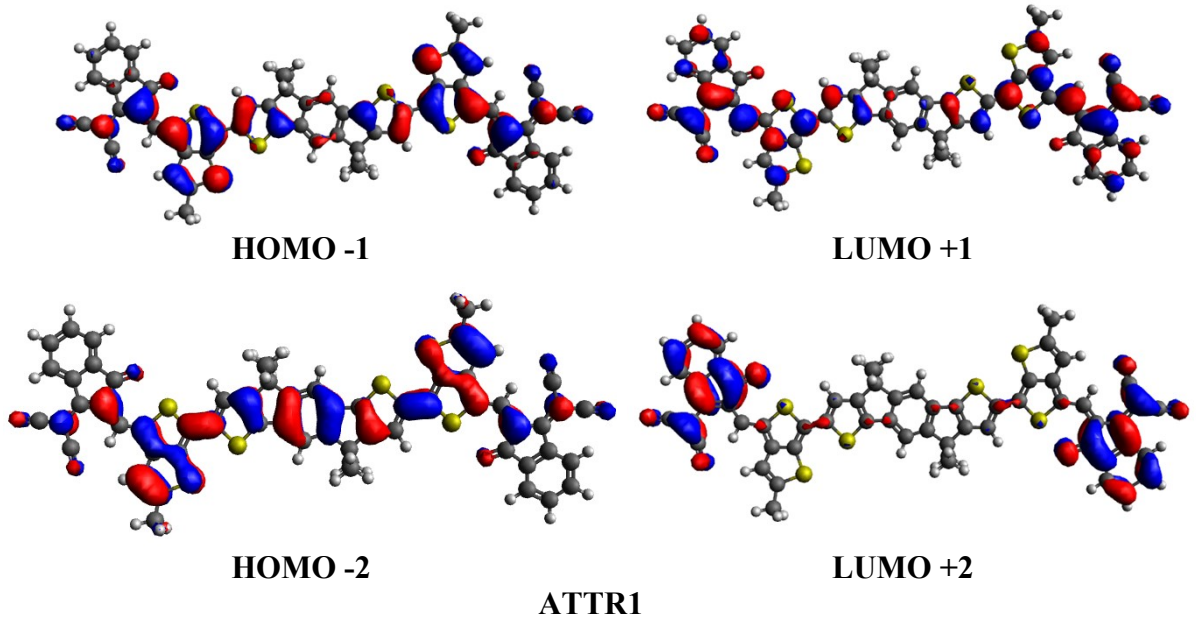
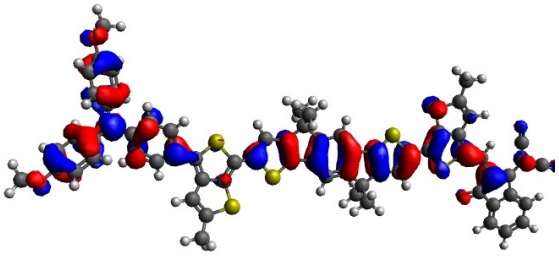


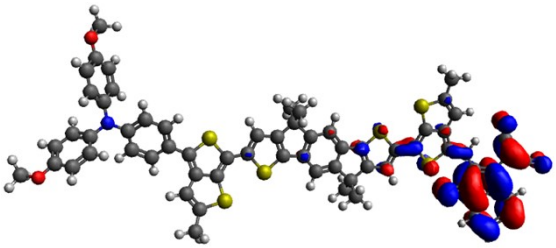
Figure S1: Optimized structures of reference compound (**ATTR1**) and designed derivatives (**ATTD2-ATTD8**).



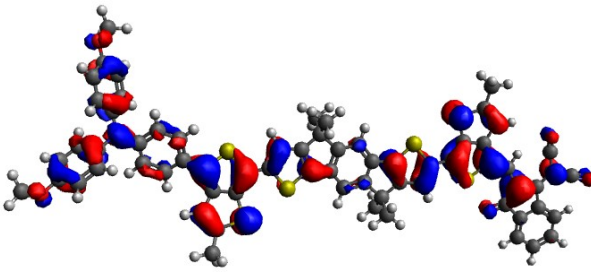
ATTR1



HOMO -1



LUMO +1



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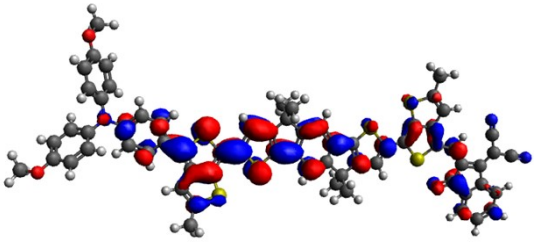
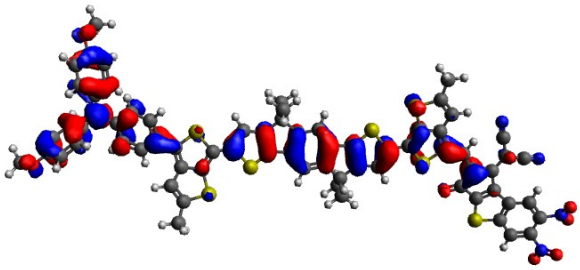


LUMO +2

ATTD2



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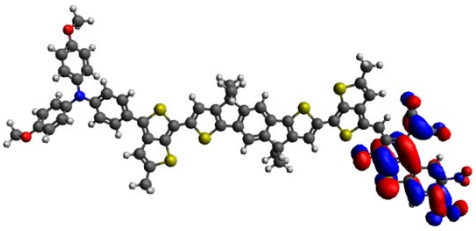

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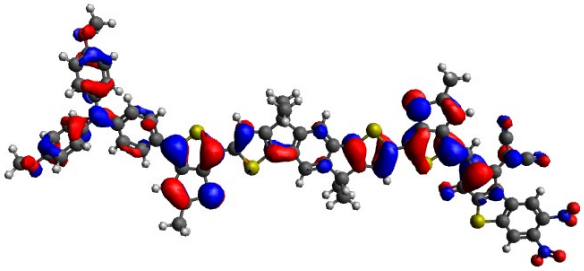

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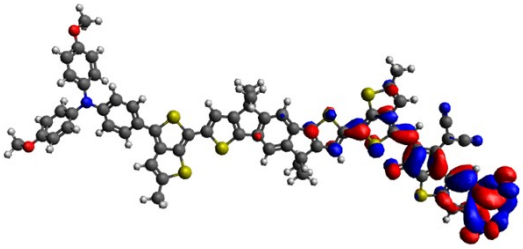
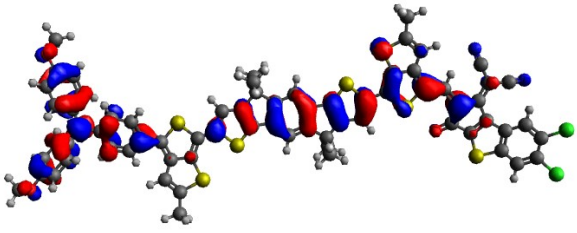


LUMO +2

ATTD3



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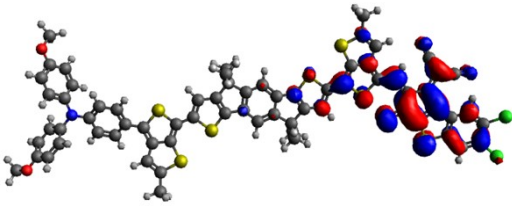
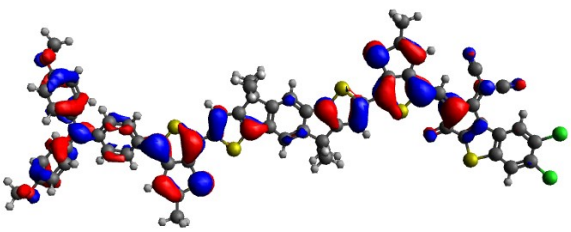
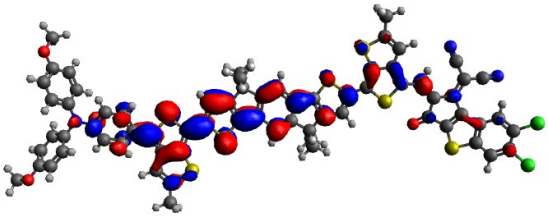


LUMO +1

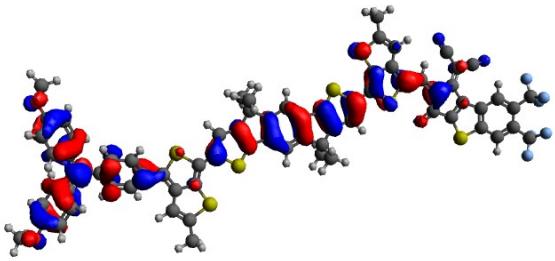


HOMO -2

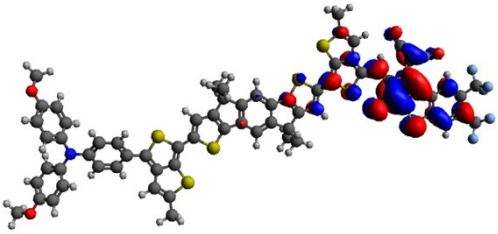


LUMO +2

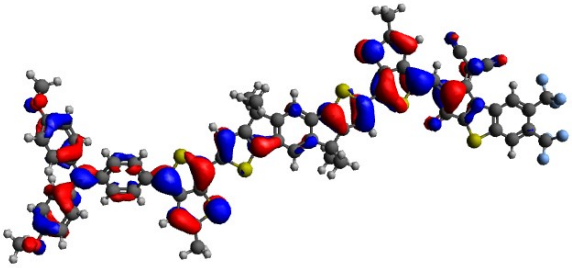
ATTD4



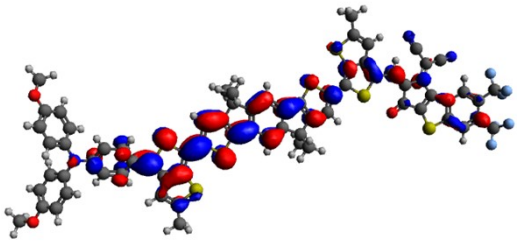
HOMO -1



LUMO +1

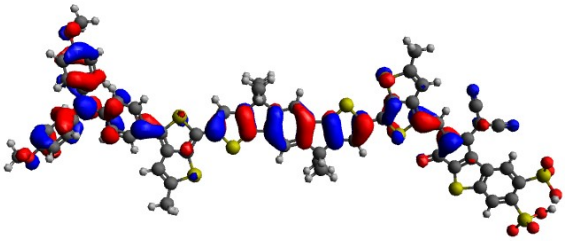


HOMO -2



LUMO +2

ATTD5



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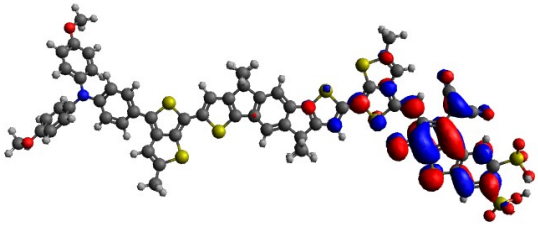
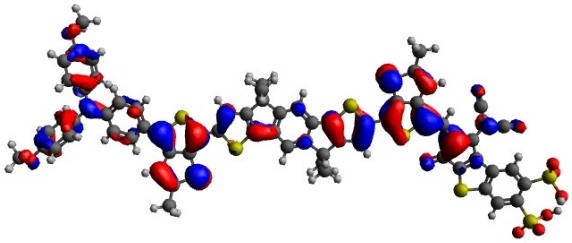
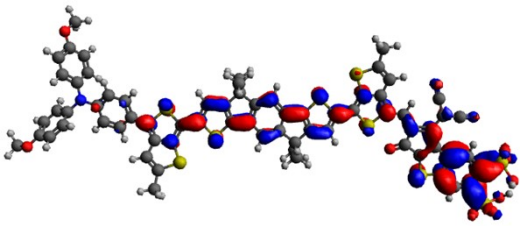


LUMO +1



HOMO -2



LUMO +2

ATTD6

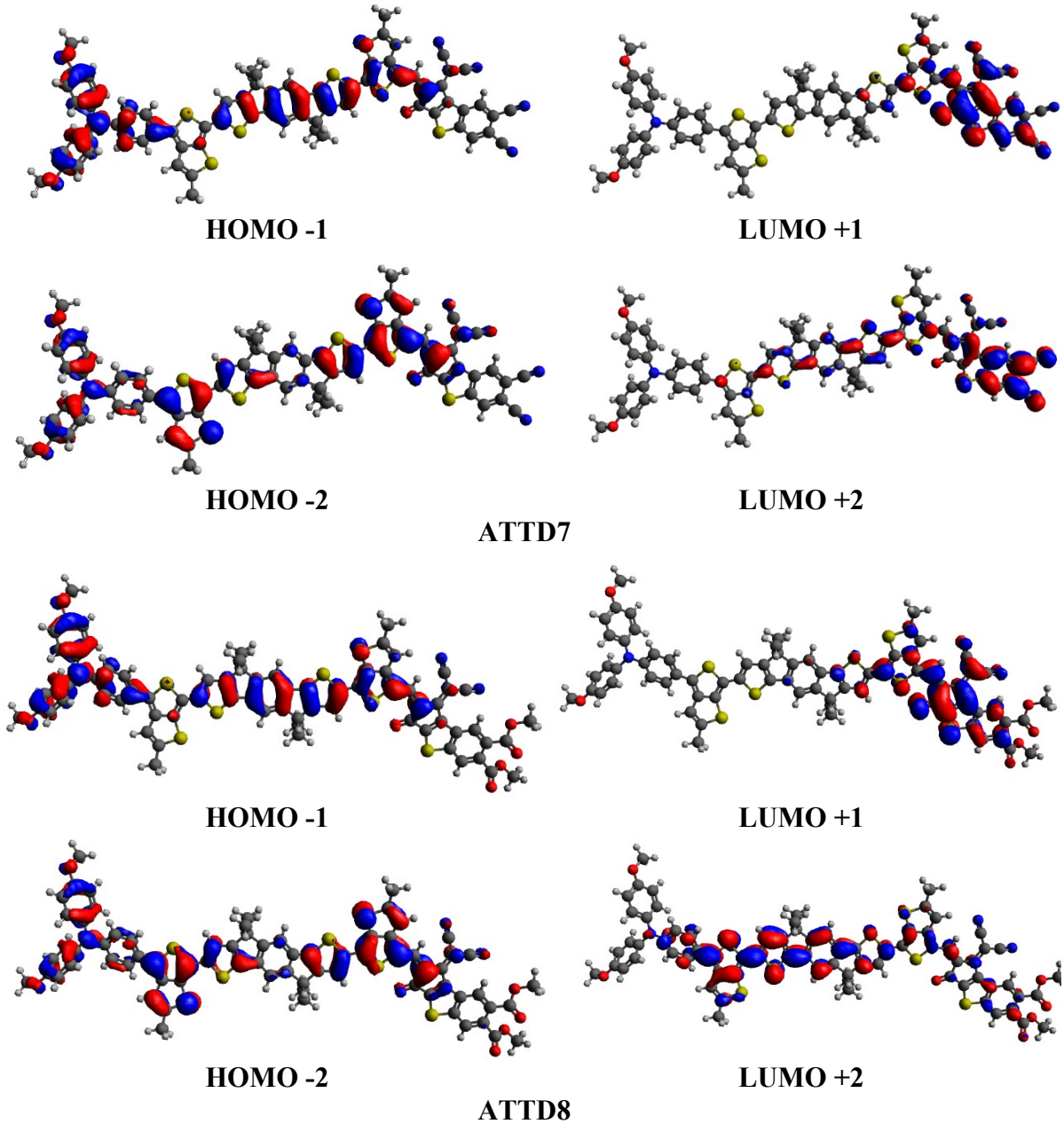
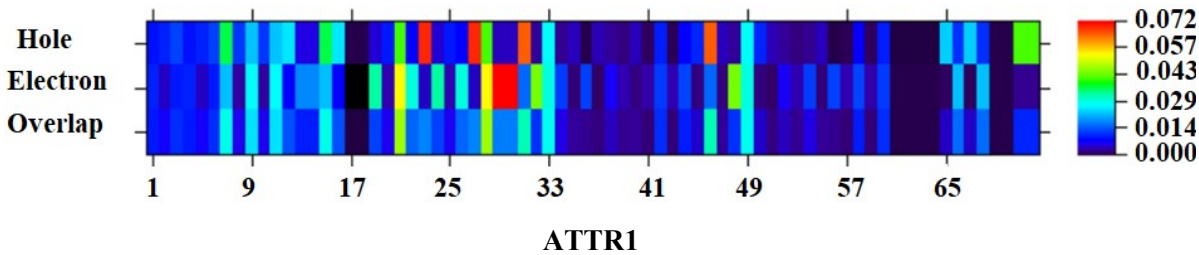
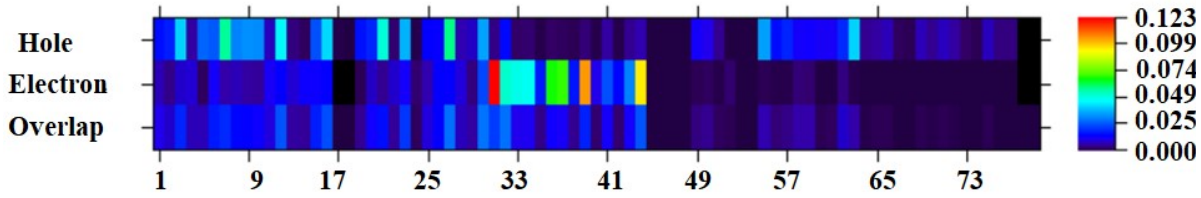
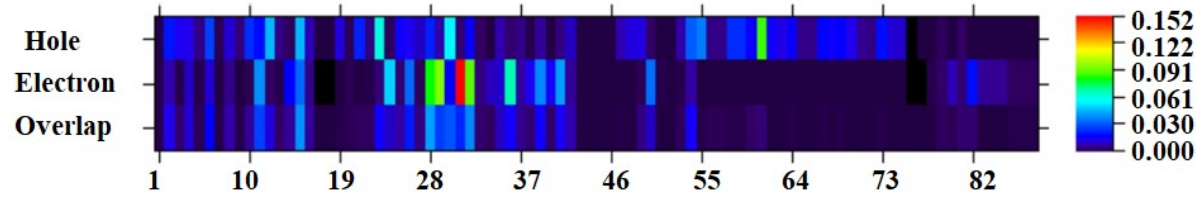


Figure S2: The pictograph of HOMO-1, LUMO+1, HOMO-2 and LUMO+2 of tailored compounds (**ATTR1** and **ATTD2-ATTD8**).

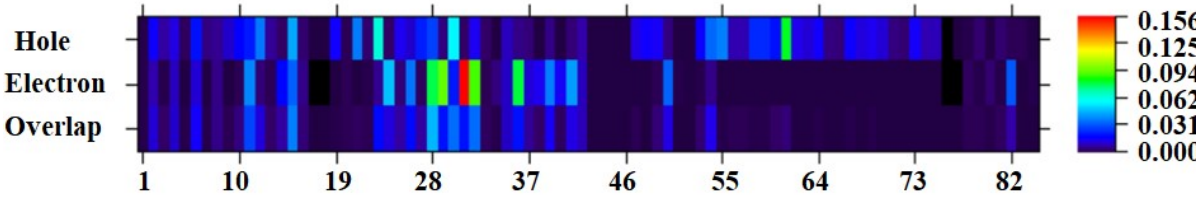




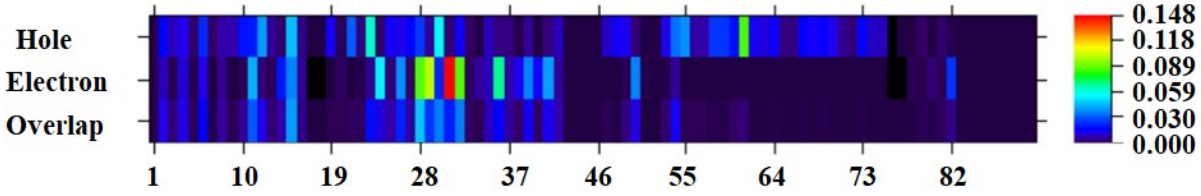
ATTD2



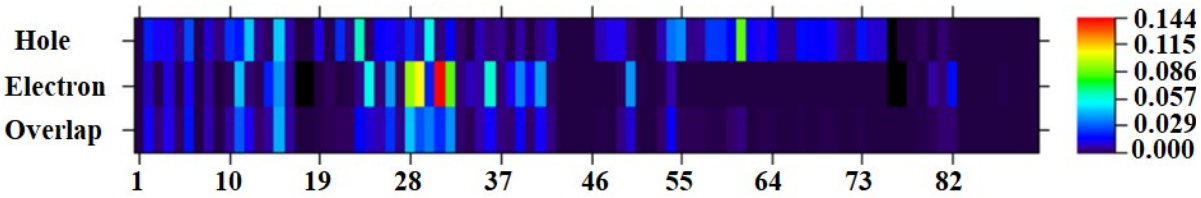
ATTD3



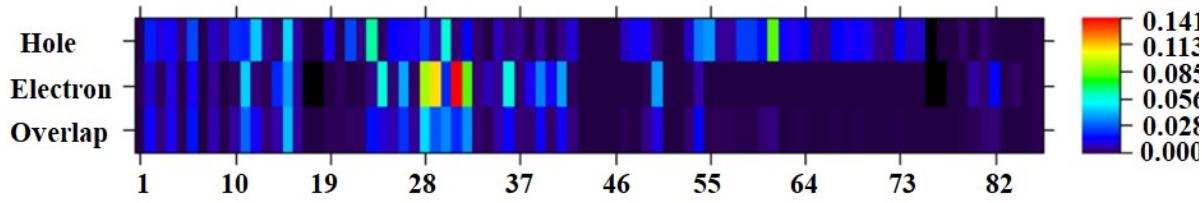
ATTD4



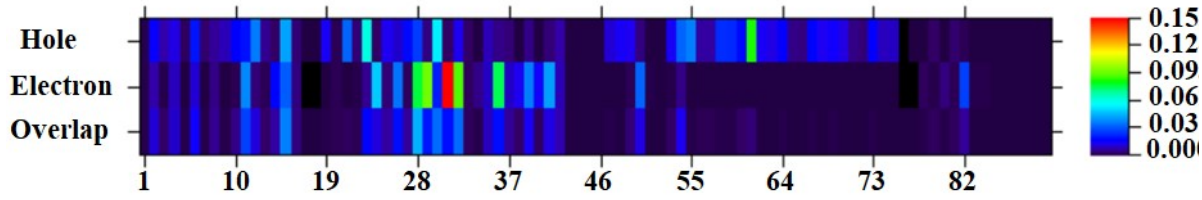
ATTD5



ATTD6

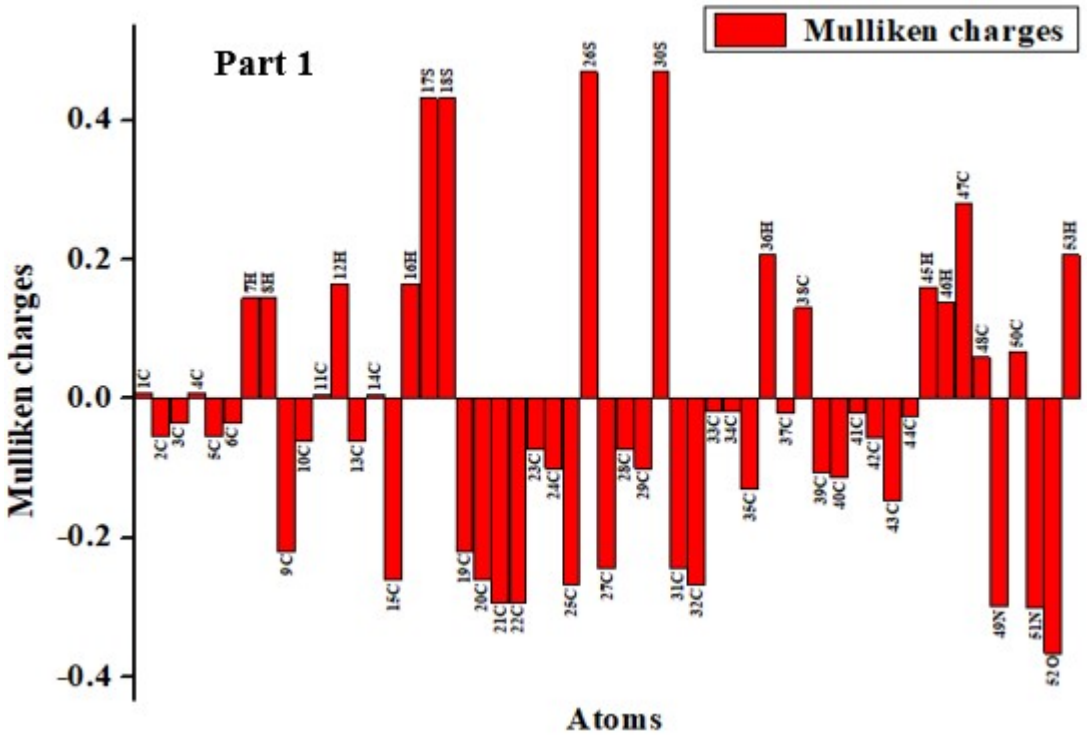


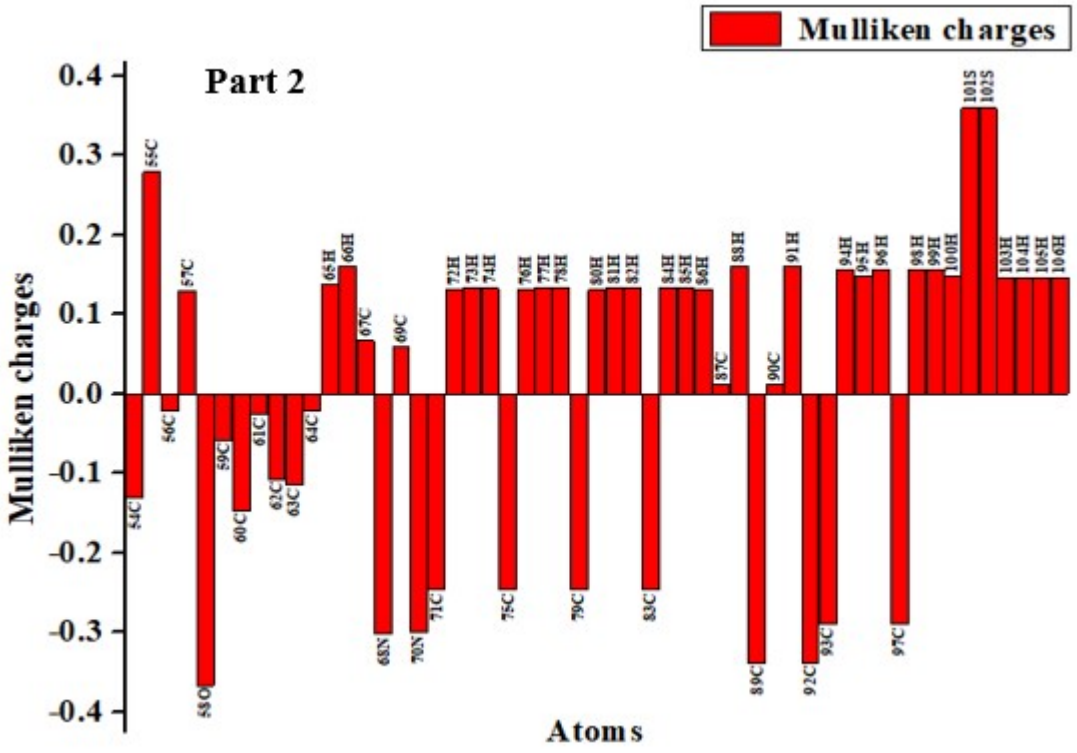
ATTD7



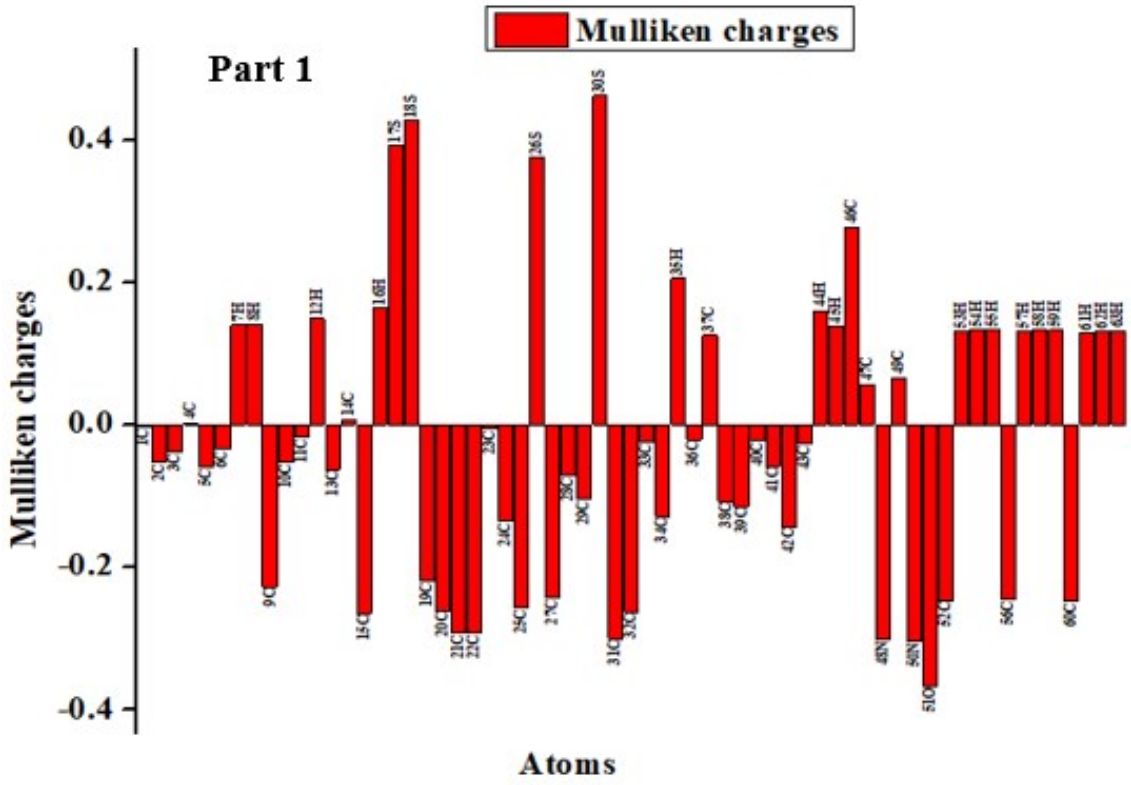
ATTD8

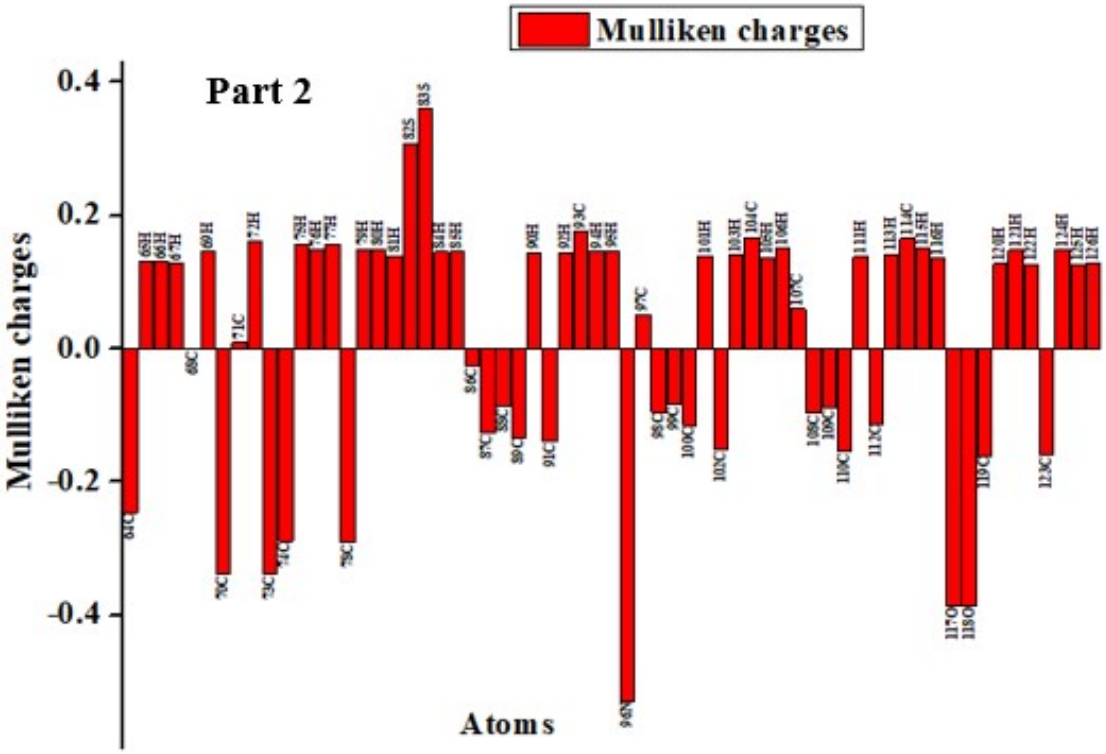
Figure S3. Pictorial representation of hole-electron transport investigation.



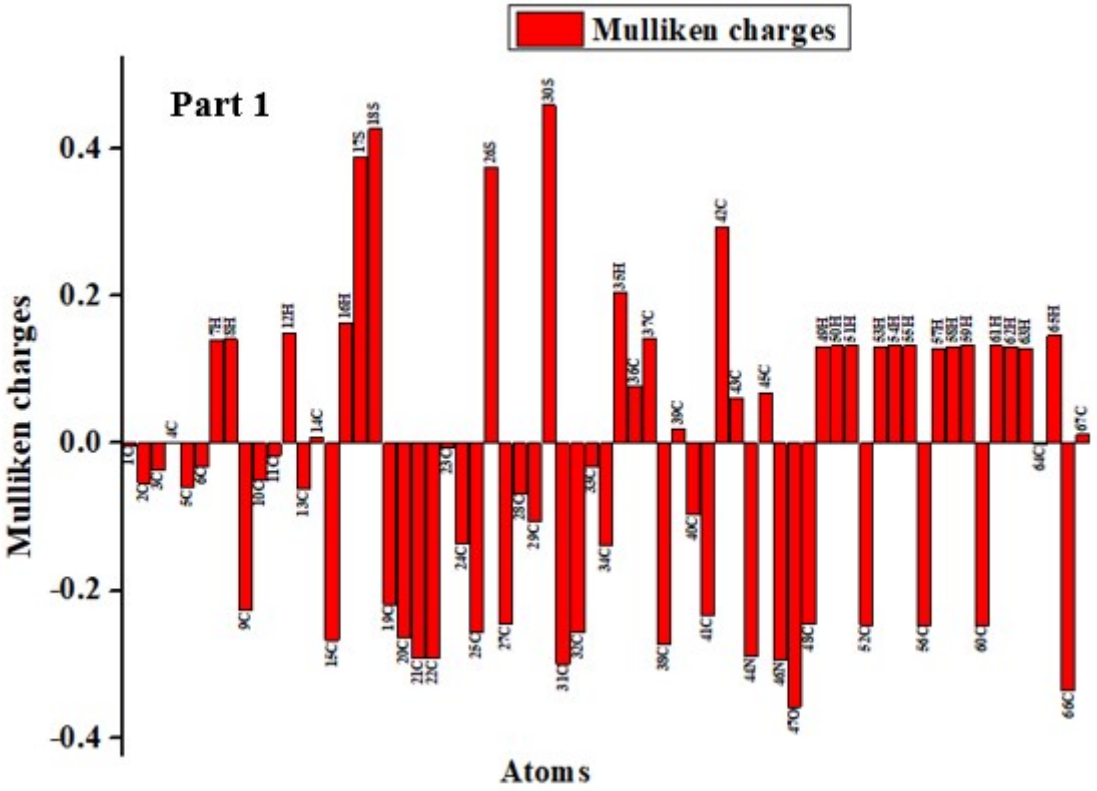

Mulliken charges
Part 2
Mulliken charges
Atoms
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
-0.4

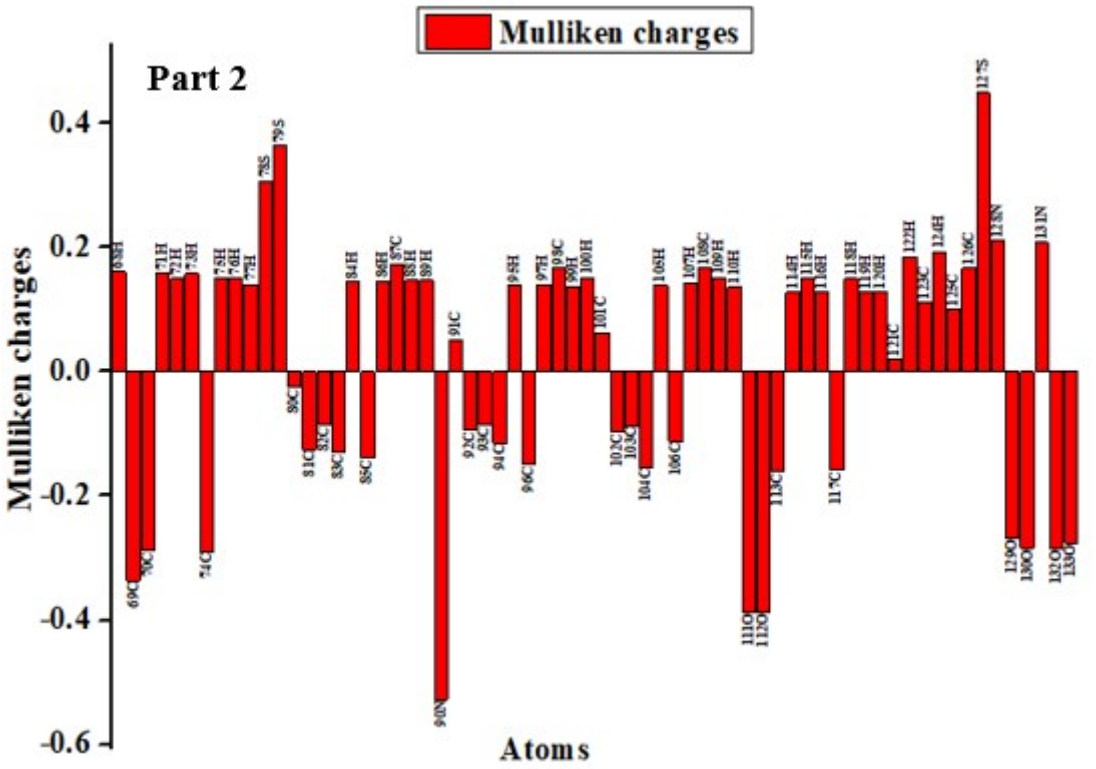
ATTR1


Mulliken charges
Part 1
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4

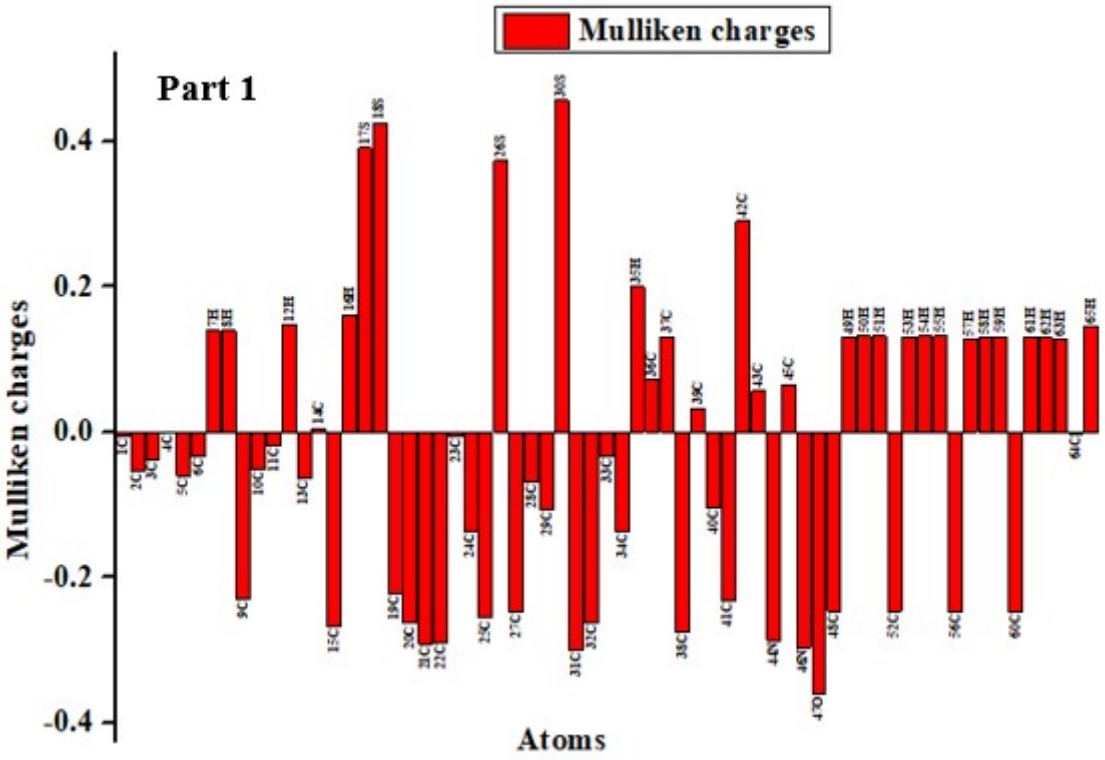

Mulliken charges
Part 2
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4

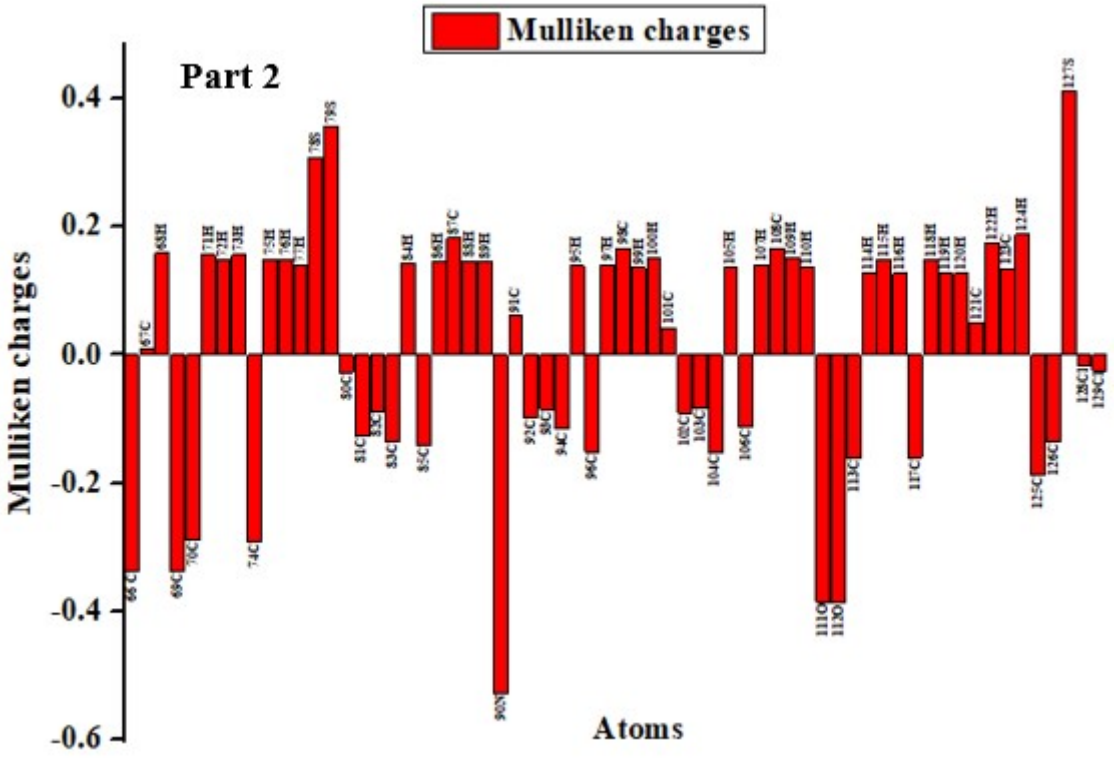
ATTD2


Mulliken charges
Part 1
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4

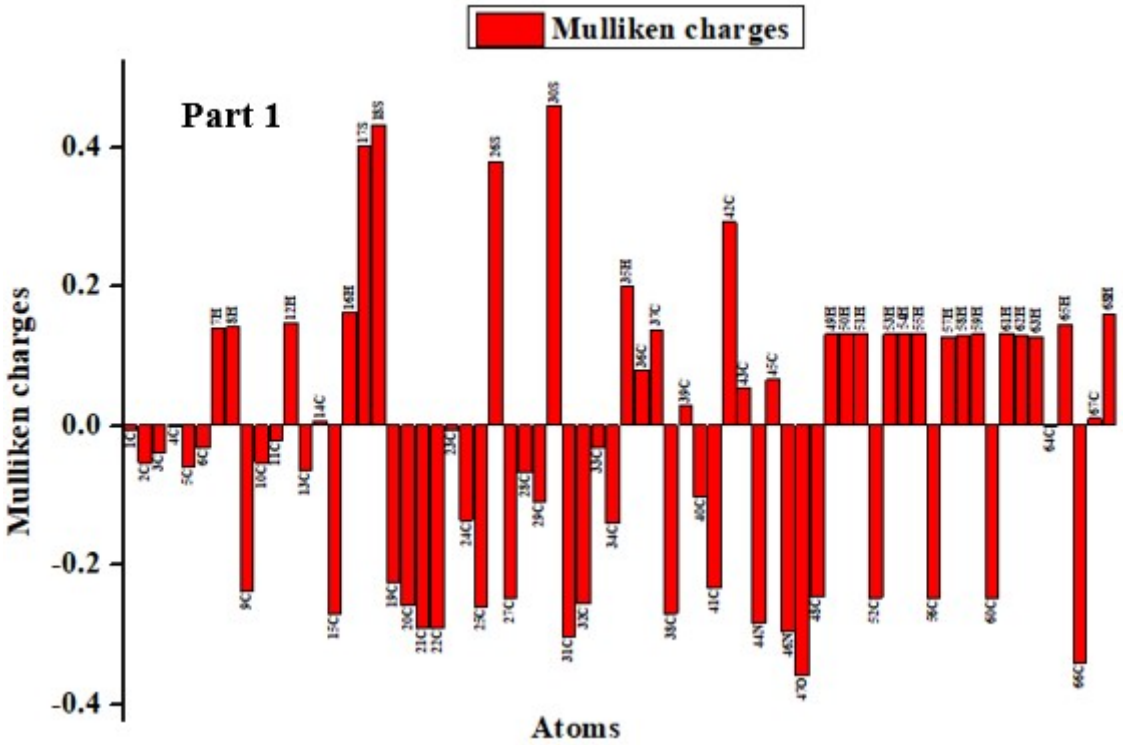

Mulliken charges
Part 2
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4
-0.6

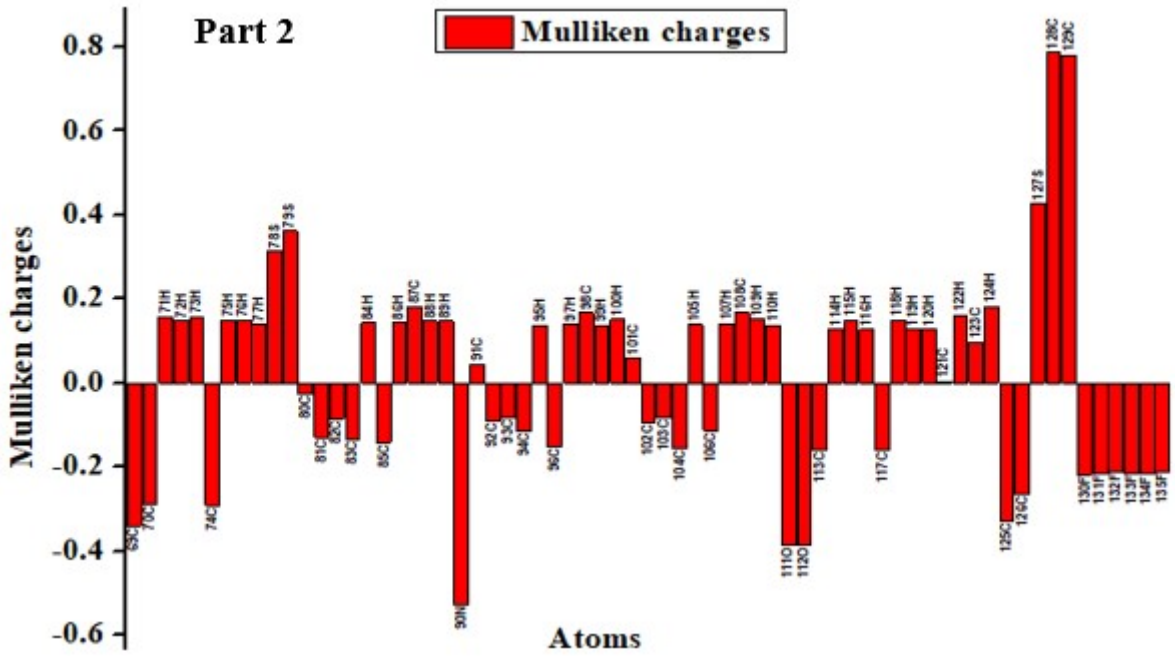
ATTD3


Mulliken charges
Part 1
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4

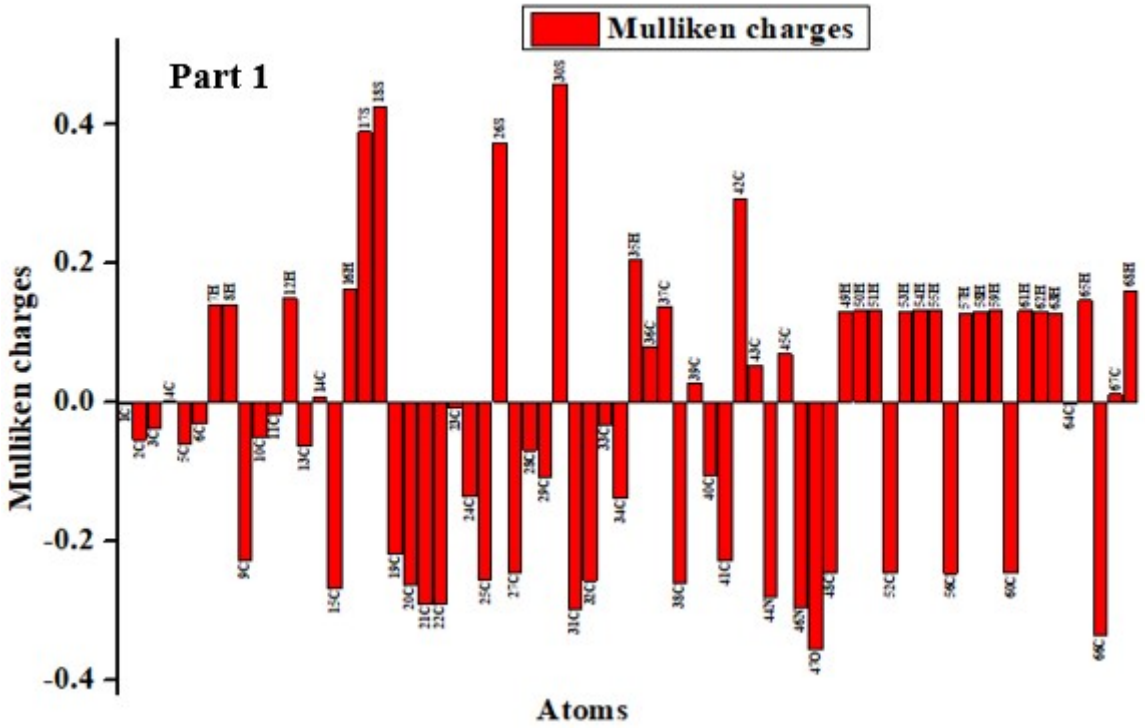

Mulliken charges
Part 2
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4
-0.6

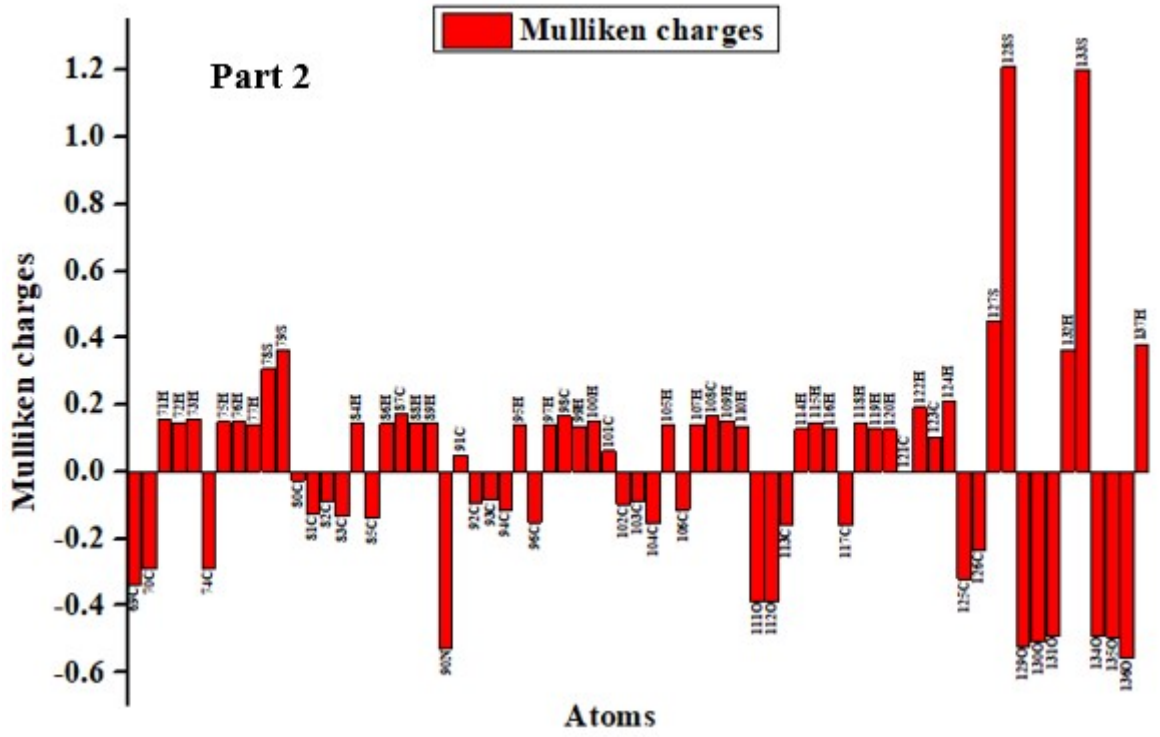
ATTD4


Mulliken charges
Part 1
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4

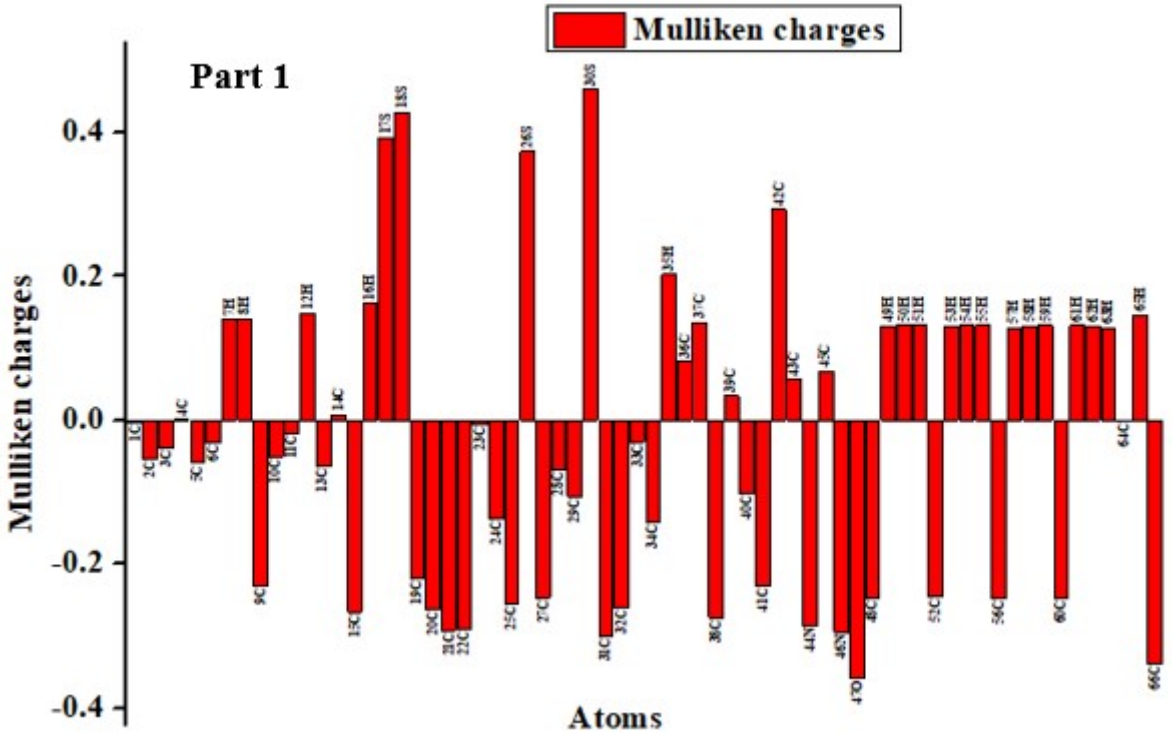

Part 2
Mulliken charges
Mulliken charges
Atoms
0.8
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6

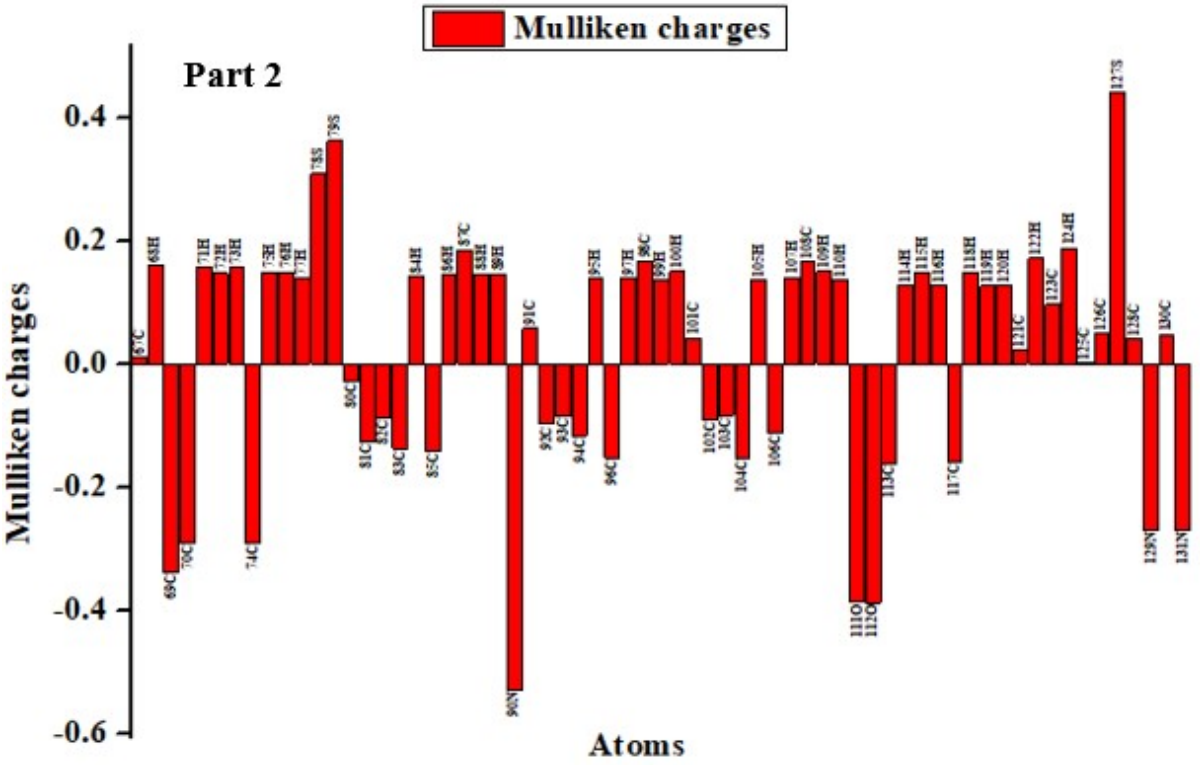
ATTD5


Part 1
Mulliken charges
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4

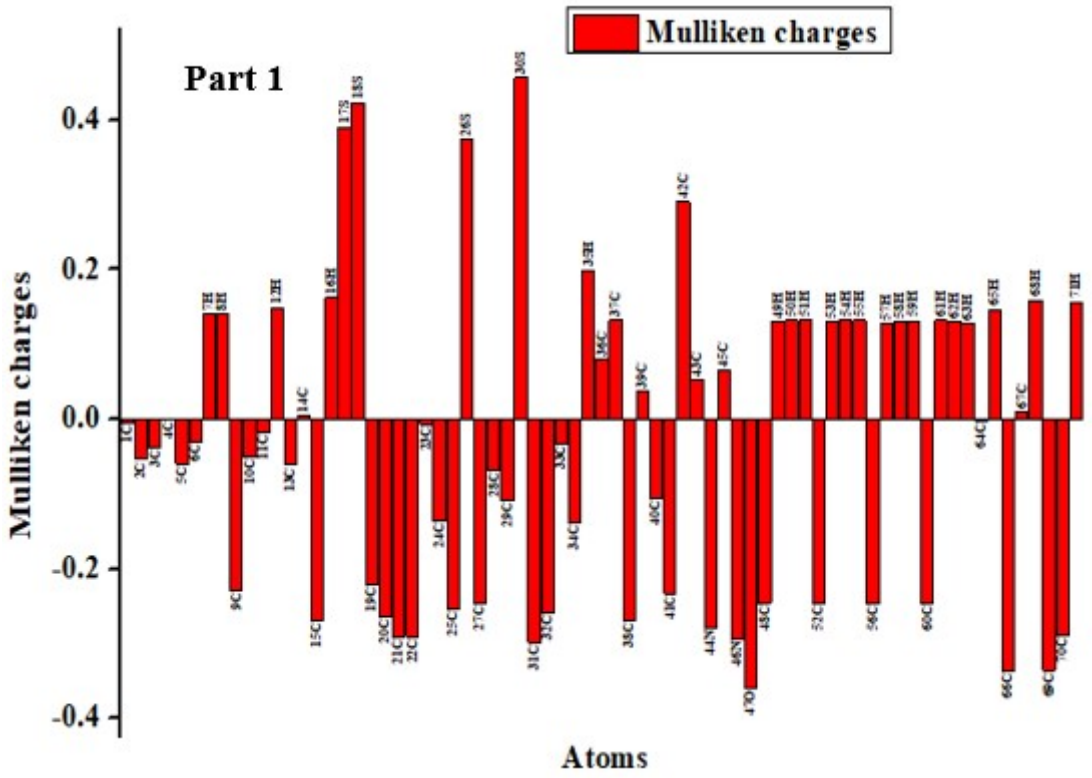

Mulliken charges
Part 2
Mulliken charges
Atoms

ATTD6


Mulliken charges
Part 1
Mulliken charges
Atoms


Mulliken charges
Part 2
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4
-0.6

ATTD7


Mulliken charges
Part 1
Mulliken charges
Atoms
0.4
0.2
0.0
-0.2
-0.4

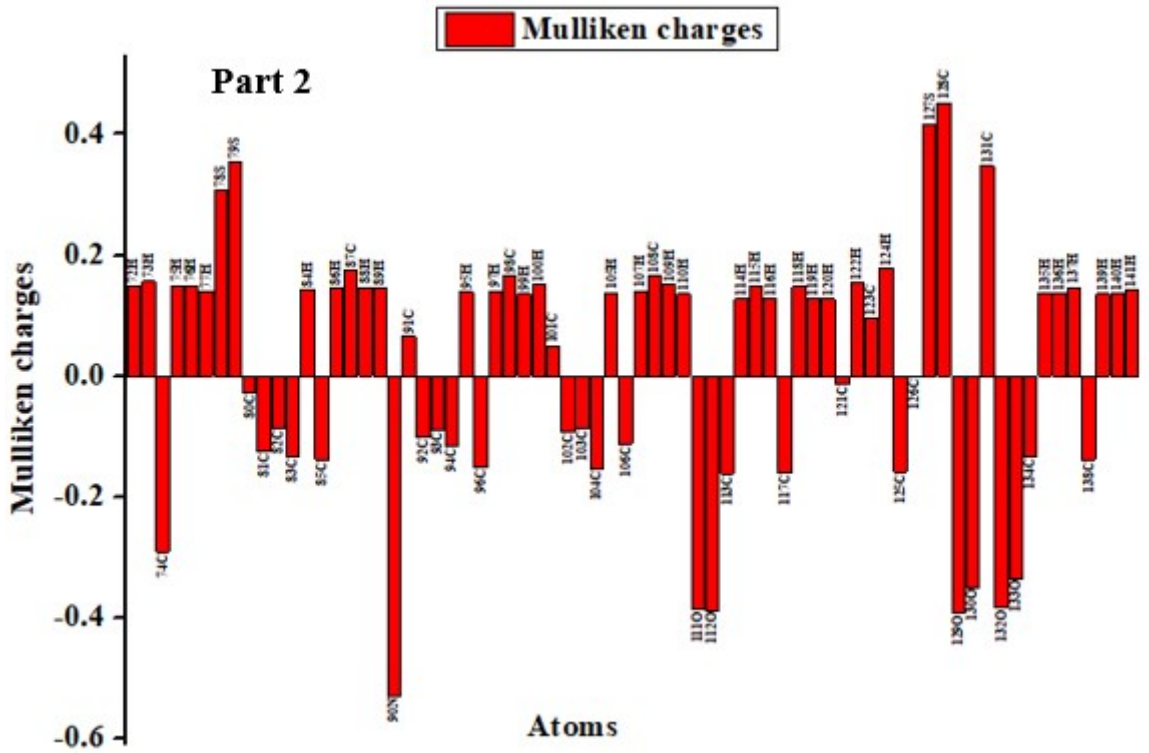


Figure S4: The graphs of Natural population analysis of **ATTR** and **ATTD2-ATTD8.**

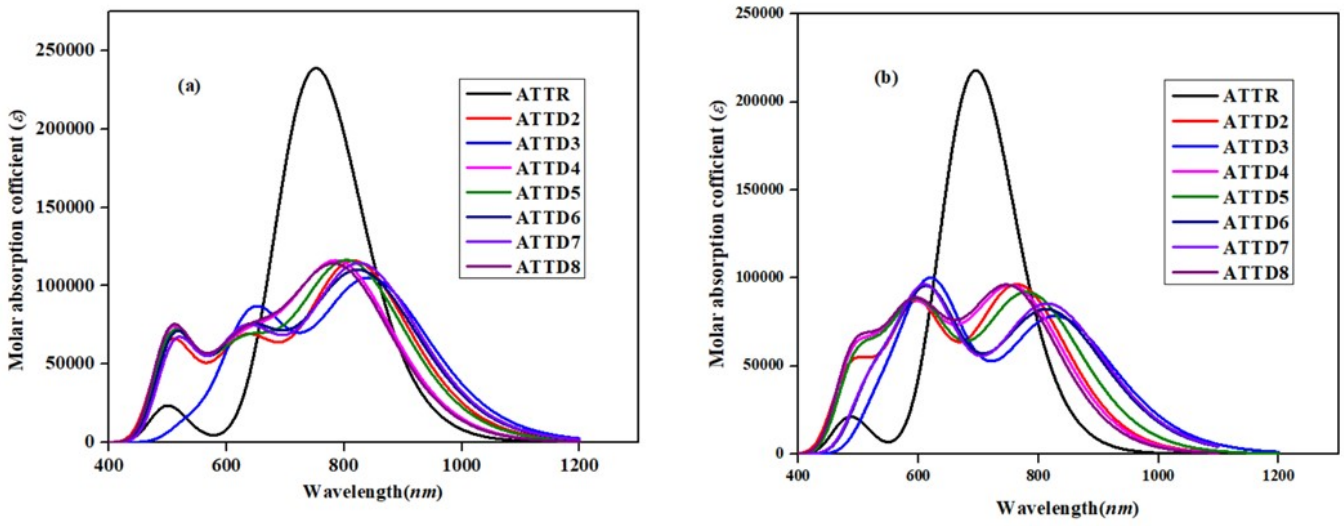
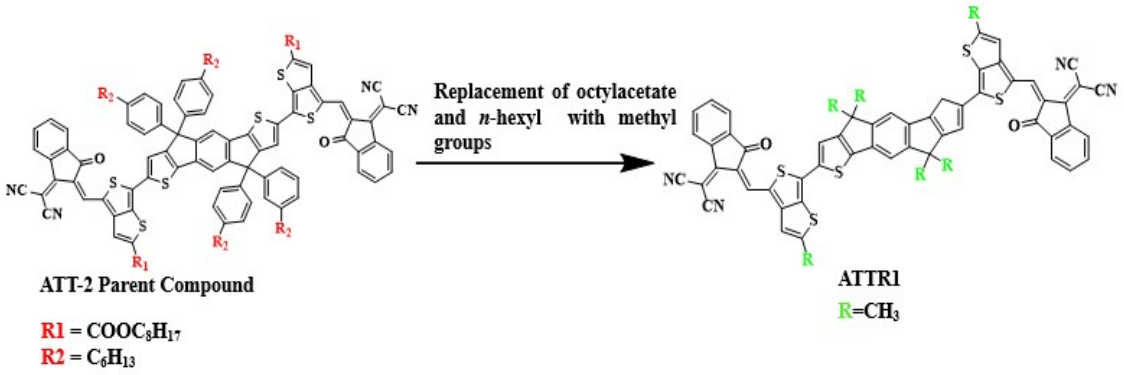
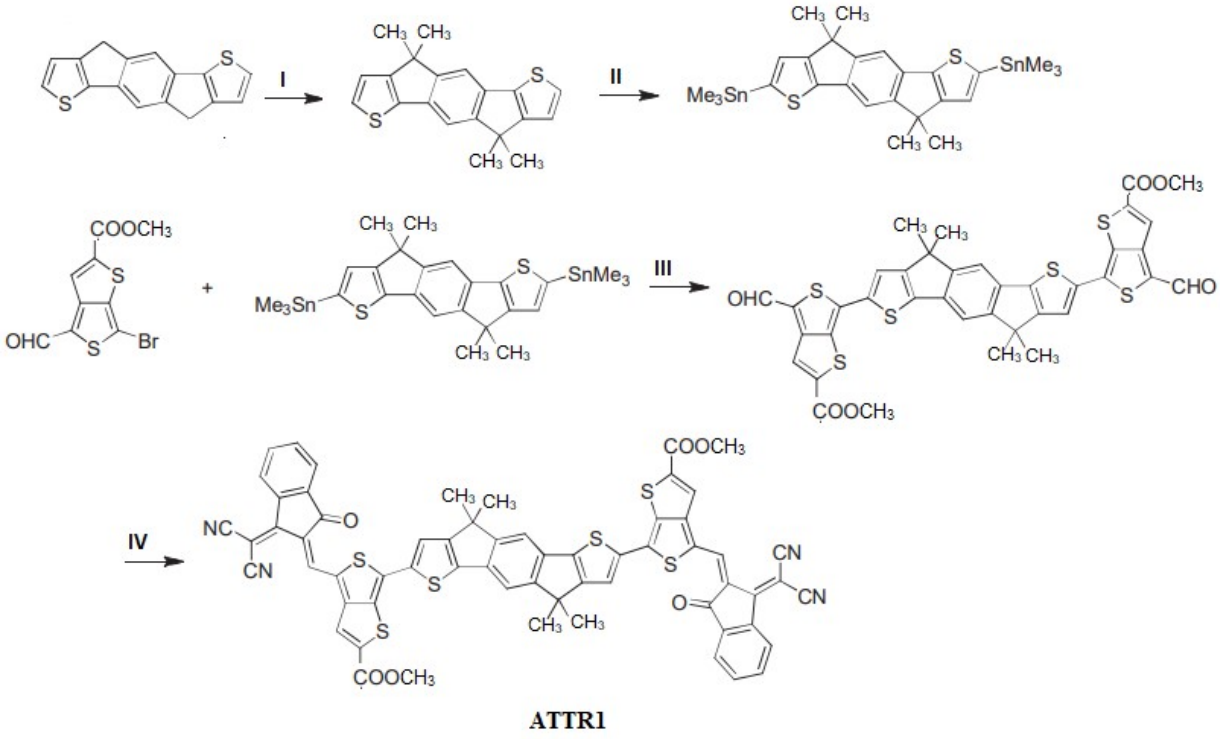


Figure S5: Absorption spectra of **ATTR** and **ATTD2-ATTD8 (a)** in chloroform and (b) in gaseous phase.

CH_3



(a)



(b)

Figure S6: Side-chain variation of parent compound **ATT-2** into a reference **ATTR1 (a),** Synthesis of reference compound **ATTR1** reagents and conditions: I) $NaOH/H_2O$, CH_3-Br, 50 wt %, II) n-BuLi, $SnMe_3CL$,THF 95% III) Pd(PPh3)4, toluene, reflux; IV) 3-(dicyanomethylidene)indan-1-one, pyridine, chloroform, reflux **(b)**